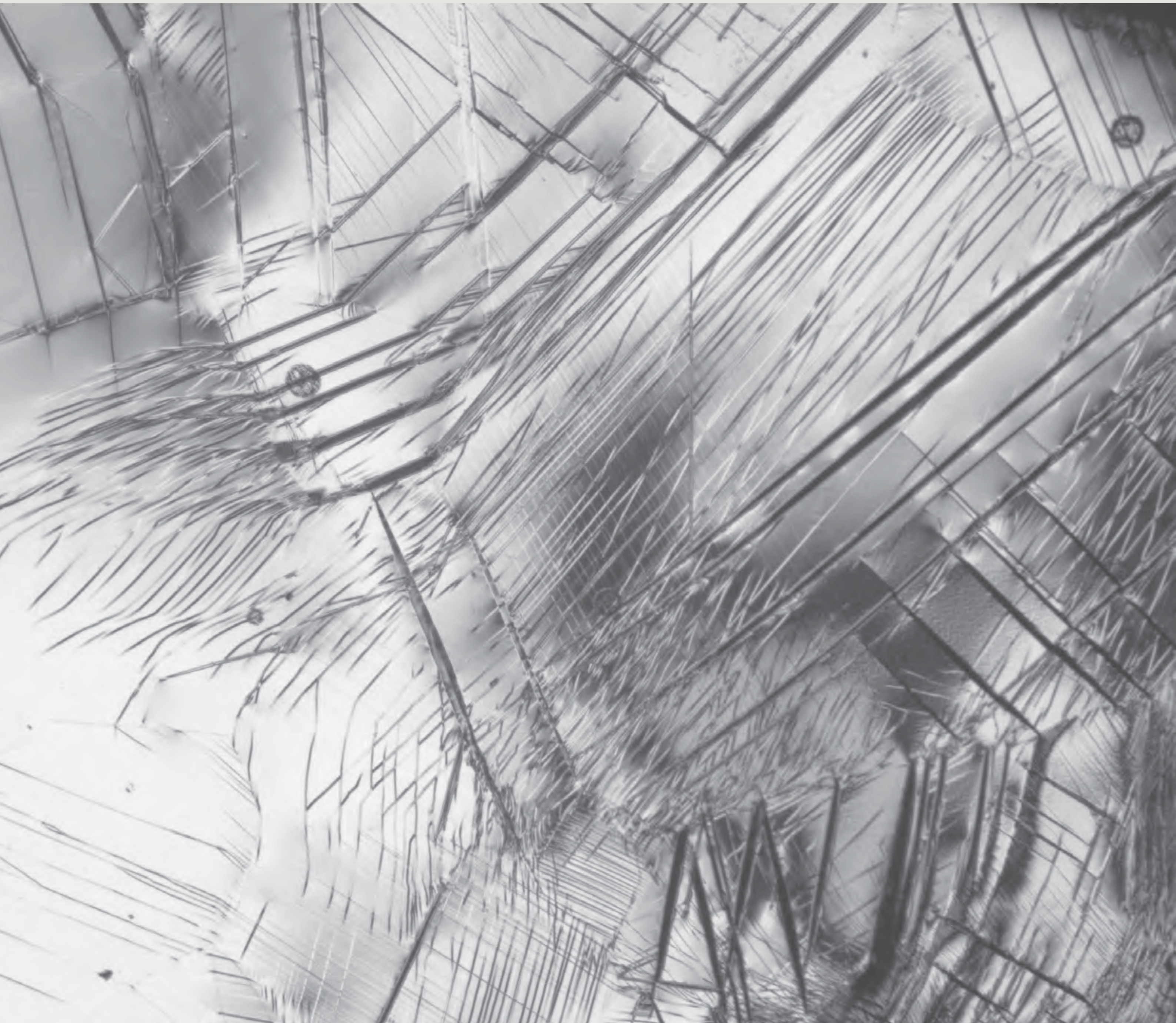
MAX-PLANCK-GESELLSCHAFT

# Scientific Report
# 2011 / 2012

Max-Planck-Institut
für Eisenforschung GmbH



Max-Planck-Institut für Eisenforschung GmbH

# Scientific Report 2011/2012

November 2012
Max-Planck-Institut für Eisenforschung GmbH
Max-Planck-Str. 1 · 40237 Düsseldorf
Germany

*Front cover*

Oxygen is one of the critical components that give rise to the excellent mechanical properties of Ti-Nb based gum metal (Ti−23Nb−0.7Ta−2Zr−1.2O at%) and its complex deformation mechanism. Yet, its role is not fully clear, for which reason an extensive project is being carried out at MPIE (see highlight article on page 113). As a part of this project, deformation structures in gum metal (Ti−22.6Nb−0.47Ta−1.85Zr−1.34O at%) are compared to those in a reference alloy that has the same chemical composition, but no oxygen (Ti−22.8Nb−0.5Ta−1.8Zr at%). The cover page shows a light microscope image of a sample of the reference alloy deformed in uniaxial tension, revealing mechanically-induced crystallographic twin steps on a priorly-polished surface (1 cm corresponds to approx. 125 µm).

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Phone: +49-211-6792-0
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*Editorship, Layout and Typesetting*
Yasmin Ahmed-Salem
Gabi Geelen
Brigitte Kohlhaas
Frank Stein

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# PREFACE

This report is part of a series documenting the scientific activities and achievements of the Max-Planck-Institut für Eisenforschung GmbH (MPIE) in 2011 and 2012. For evaluation purposes some main trends are described over the past 6 years.

MPIE conducts basic research on structural materials, specifically steels, for nearly one century, considering their complex chemical-physical synthesis, characterisation and properties, as well as their use in systemic components. Projects are characterized by a highly interdisciplinary approach including close interfacing between experiment and theory.

Through its research on structural materials the Institute plays a central role in enabling progress in the fields of mobility (e.g. steels and soft magnets for light weight hybrid vehicles), energy (e.g. efficiency of thermal power conversion through better high temperature alloys), transport (e.g. Ni-base alloys for plane turbines), infrastructure (e.g. steels for large infrastructures, e.g. wind turbines and chemical plants) and safety (e.g. nanostructured bainitic steels for gas pipelines). A close match between knowledge-oriented and pre-competitive basic research on the one hand and commercial relevance on the other hand is an important cornerstone of this concept. With its system-oriented research agenda and its 50% institutional co-sponsoring by industry, the Institute is a unique example of public private partnership both for the Max Planck Society and for the European industry.

The departments jointly pursue a number of cross-disciplinary research branches covering Materials Design (simulation, synthesis, combinatorial materials design), Materials Analysis (structure, chemistry, defects), Materials Processing (thermomechanical treatment, forming, joining, coating), and Materials Properties (mechanical, stability, function). In many of these areas the institute holds a position of international scientific leadership, particularly in multiscale materials modeling; surface science; metallurgical alloy design; and characterization from atomic to macroscopic scales of complex engineering materials.

Profound strengthening of the institute's scientific profile is also achieved by the close cooperation with R. Kirchheim (materials physics and atom scale characterization; University of Göttingen) who is an external scientific member of the Max-Planck Society and with G. Eggeler (high temperature alloys and energy-related materials; Ruhr-University Bochum) who is a fellow of the Max-Planck Society. With both colleagues a number of joint projects are being pursued (e.g. exploring the limits of strength in Fe−C systems; hydrogen-propelled materials and systems; defectant theory; creep of superalloys; atomic scale analysis of interfaces in superalloys).

The institute hosts about 270 people, the majority being scientists. As only 120 employees are funded by the basic budget provided by the shareholders of the institute, nearly 150 additional scientists work at the institute supported by extramural sources. This strong contribution of third-party funds and its balance between fundamental and applied science gives the institute a singular position within the Max-Planck Society.

The increasing number of co-operations with key industry partners has provided further extramural momentum to the dynamic growth of the institute during the past two years. Besides the well established links to material companies in the fields of structural alloy design (bulk and surface), advanced characterization methods in steel development, surface functionalization, and computational materials science, new exiting industrial co-operations are currently being developed 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 that deals with complex materials in a more holistic context of including complicated engineering systems, loading, and environmental conditions into advanced materials science and engineering projects. 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 report is structured into IV parts:

- *Part I* presents the organization of the institute including a short section on recent scientific developments, new scientific groups, large network activities, and new scientific laboratories at the institute.

- *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 summarise major recent scientific achievements in the four areas of common interest of the institute ‘New Structural Materials’, ‘Microstructure-Related Materials Properties’, ‘Stability of Surfaces and Interfaces’, and ‘Scale-Bridging Simulation of Materials’.

- *Part IV* summarises some statistically relevant information about the institute.

Dierk Raabe, Chairman of the executive board
Düsseldorf, November 2012

# CONTENTS

## PART I. THE INSTITUTE 7

## PART II. THE DEPARTMENTS 33

## PART III. INTER-DEPARTMENTAL RESEARCH ACTIVITIES - SELECTED HIGHLIGHTS 99

## PART IV. GENERAL INFORMATION AND STATISTICS 153

# PART I.

# THE INSTITUTE

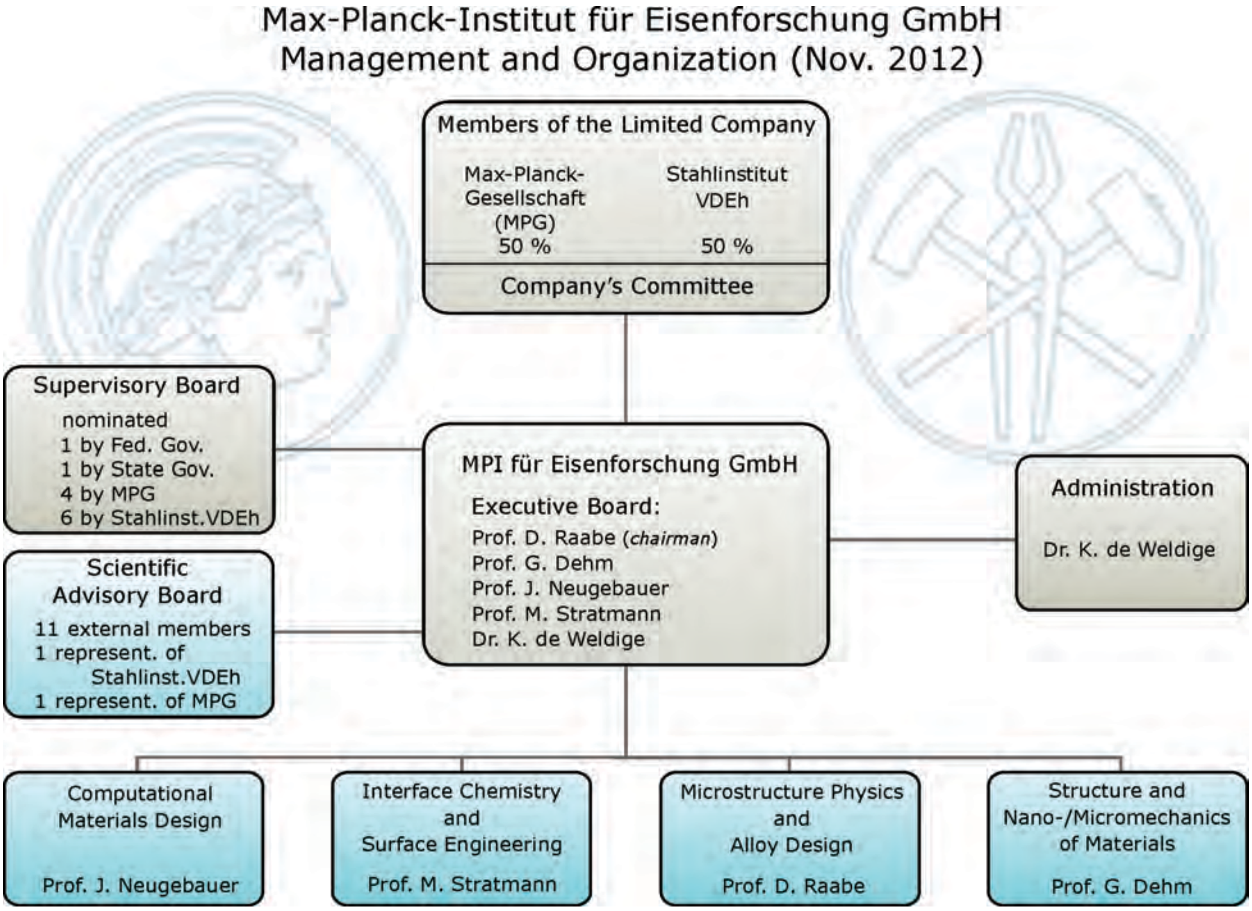
# Management of the Institute

The Max-Planck-Institut für Eisenforschung (MPIE) is a joint venture between the Max Planck Society and the Steel Institute VDEh. Since half of 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 institute 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 institute 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 the institute has operated on the legal basis of a limited liability company (GmbH) and its budget is equally 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 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 institute'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.



# Scientific Organization

The institute devotes its research to iron, steel and related materials. In addition to the development of new materials, the institute focuses on the physical and chemical processes and reactions which are of importance for material production, processing, materials characterization and properties.

The institute is divided into the following 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): aspects of environmentally accelerated degradation of surfaces and interfaces like 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

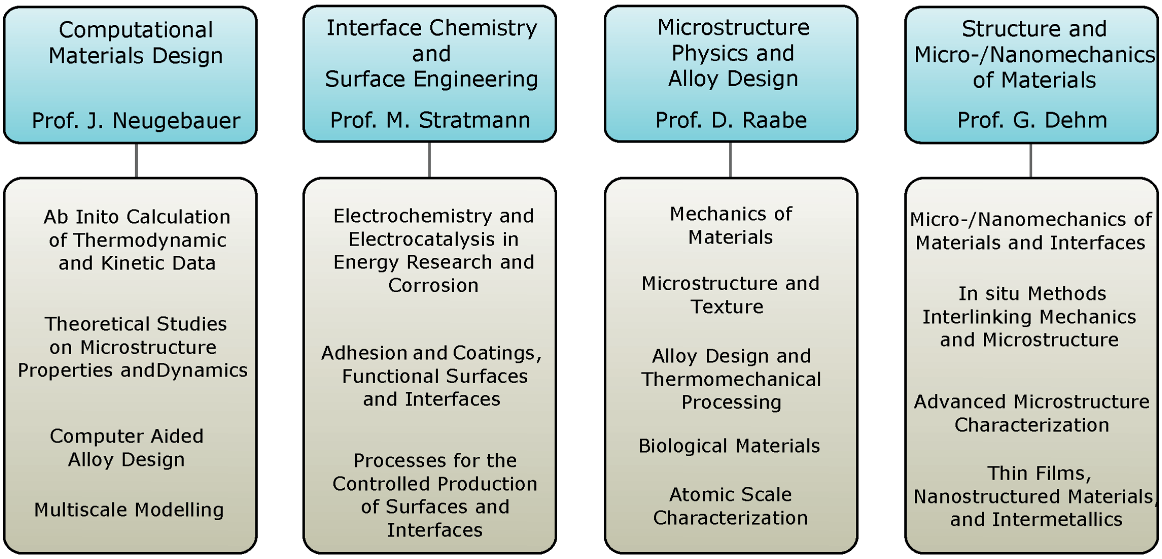
The main scopes of the departments are summarized in the figure below.

Each department is subdivided into research groups which are typically managed by group heads. The figure on the right side 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 different departments. In concerted activities, scientific and technological breakthroughs in highly competitive research areas are achieved. Selected scientific highlights including such inter-departmental research activities are described in Part III which is divided into the four topics

- New Structural Materials
- Microstructure-Related Materials Properties
- Stability of Surfaces and Interfaces
- Scale-Bridging Simulation of Materials

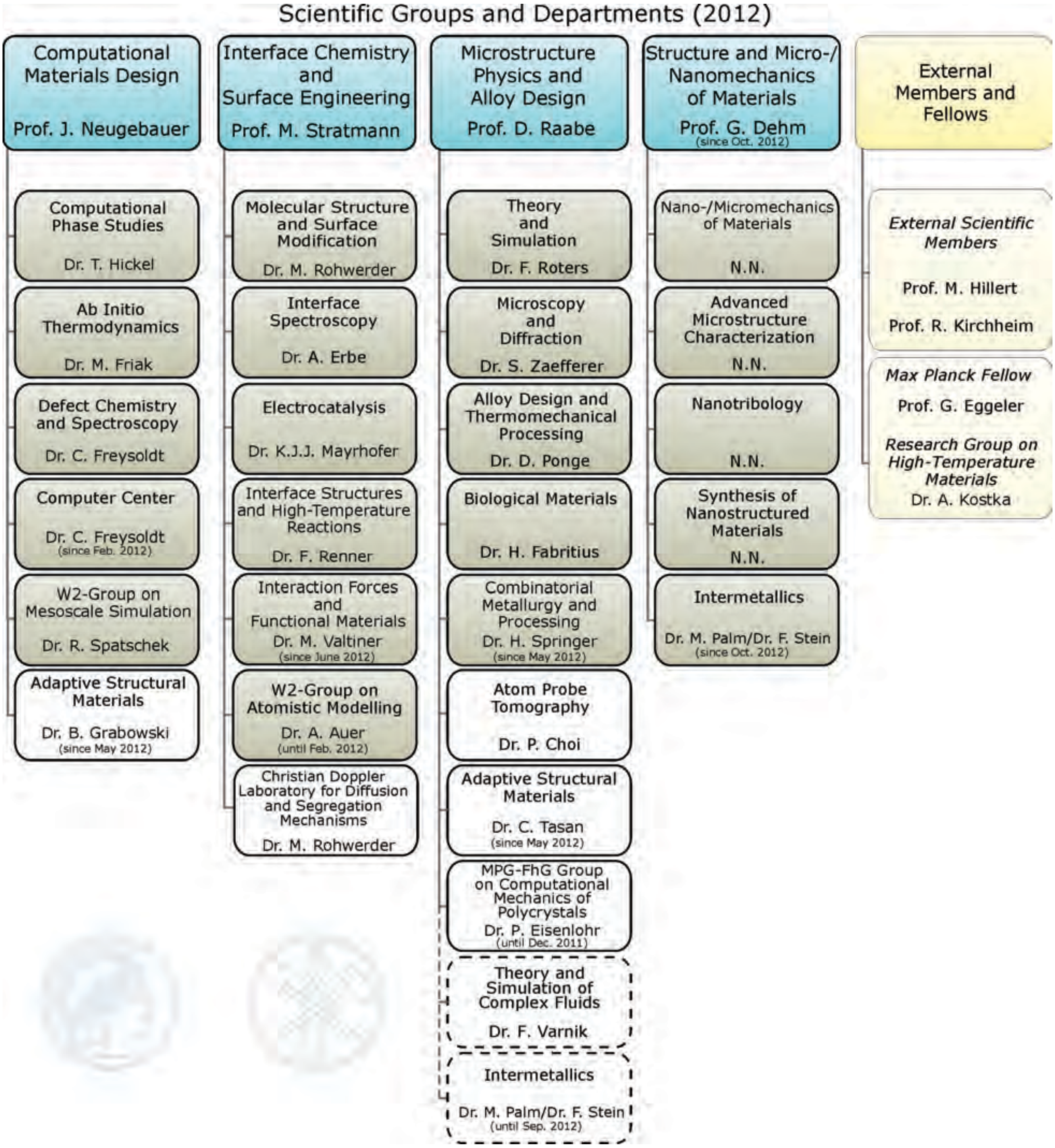
Scientific Scopes of the Departments



For each of these four 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 two years.

In summary, the research within the institute 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 and a homogeneous research profile.

Service groups provide the scientific departments with valuable experimental expertise. These services include the production 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 and a computer network centre.



Scientific Groups and Departments (2012)

**Computational Materials Design**
**Prof. J. Neugebauer**
- Computational Phase Studies – Dr. T. Hickel
- Ab Initio Thermodynamics – Dr. M. Friak
- Defect Chemistry and Spectroscopy – Dr. C. Freysoldt
- Computer Center – Dr. C. Freysoldt (since Feb. 2012)
- W2-Group on Mesoscale Simulation – Dr. R. Spatschek
- Adaptive Structural Materials – Dr. B. Grabowski (since May 2012)

**Interface Chemistry and Surface Engineering**
**Prof. M. Stratmann**
- Molecular Structure and Surface Modification – Dr. M. Rohwerder
- Interface Spectroscopy – Dr. A. Erbe
- Electrocatalysis – Dr. K.J.J. Mayrhofer
- Interface Structures and High-Temperature Reactions – Dr. F. Renner
- Interaction Forces and Functional Materials – Dr. M. Valtiner (since June 2012)
- W2-Group on Atomistic Modelling – Dr. A. Auer (until Feb. 2012)
- Christian Doppler Laboratory for Diffusion and Segregation Mechanisms – Dr. M. Rohwerder

**Microstructure Physics and Alloy Design**
**Prof. D. Raabe**
- Theory and Simulation – Dr. F. Roters
- Microscopy and Diffraction – Dr. S. Zaefferer
- Alloy Design and Thermomechanical Processing – Dr. D. Ponge
- Biological Materials – Dr. H. Fabritius
- Combinatorial Metallurgy and Processing – Dr. H. Springer (since May 2012)
- Atom Probe Tomography – Dr. P. Choi
- Adaptive Structural Materials – Dr. C. Tasan (since May 2012)
- MPG-FhG Group on Computational Mechanics of Polycrystals – Dr. P. Eisenlohr (until Dec. 2011)
- Theory and Simulation of Complex Fluids – Dr. F. Varnik
- Intermetallics – Dr. M. Palm/Dr. F. Stein (until Sep. 2012)

**Structure and Micro-/Nanomechanics of Materials**
**Prof. G. Dehm** (since Oct. 2012)
- Nano-/Micromechanics of Materials – N.N.
- Advanced Microstructure Characterization – N.N.
- Nanotribology – N.N.
- Synthesis of Nanostructured Materials – N.N.
- Intermetallics – Dr. M. Palm/Dr. F. Stein (since Oct. 2012)

**External Members and Fellows**
- *External Scientific Members* – Prof. M. Hillert, Prof. R. Kirchheim
- *Max Planck Fellow* – Prof. G. Eggeler
- *Research Group on High-Temperature Materials* – Dr. A. Kostka

# Recent Developments

In the reporting period 2011/12 several major scientific and administrative developments occurred which further strengthen the scientific profile of the institute:

The institute appointed Prof. G. Dehm as director and executive for a new department on the ‘Structure and Nanomechanics of Materials’. The department opened in October 2012 and is devoted to nano- and micromechanics, *in situ* electron optical characterisation, quantitative nanotribology, synthesis of nano-structured, and high-temperature intermetallic materials. The new department complements the activities of the existing departments on Microstructure Physics and Alloy Design (D. Raabe), Interface Chemistry and Surface Engineering (M. Stratmann), and Computational Materials Design (J. Neugebauer). Together, the four departments cover a broad range of state-of-the-art expertise and tools on alloy design, nano-structure oriented process design, electrochemistry and quantum mechanics to design, synthesize, and analyze complex structural materials.

Furthermore, a new research group on ultra-high resolution analytical electron microscopy will be opened by Prof. C. Scheu from LMU. This new initiative will start in fall 2013. It will mainly interact with the groups of *in situ* microscopy in the department of G. Dehm and atom probe tomography in the department of D. Raabe.

In the reporting period also a number of new research groups have been initiated and started. In the MA department H. Springer built up a group on Combinatorial Materials Synthesis and Processing. The main focus of the group is the development of new metallurgical tools and methods for a combinatorial high-throughput approach (‘steel plant in a box’) that allows to test large phase and property spaces of complex alloys such as steels.

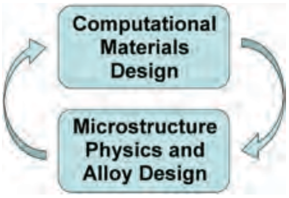
In May 2012 a research group on “Adaptive Structural Materials” started with the aim to develop next-generation high-strength and high-ductility metallic materials. A unique feature of the group is that it is headed by two heads, an experimentalist (C. Tasan) and a theoretician (B. Grabowski), thus ideally combining highly advanced experimental and theoretical expertise in the MA and CM department. Opening this group became possible by an ERC grant that had been jointly awarded to D. Raabe and J. Neugebauer.

In June 2012, M. Valtiner became head of the group "Interaction Forces and Functional Materials" in the GO department. The focus of the new group is on adhesion, friction and interfacial forces, and their utilization for making new and/or better and especially energy-saving, energy efficient, cheaper, or longer lasting smart materials, interfaces and thin films for application in structural and functional materials.

On the administrative-structural side, the institute appointed Dr. K. de Weldige as head of administration and business executive. With his background in science, finances, and administration he provides an ideal link between the scientific and administrative units in the institute and will ensure an even closer collaboration between MPIE and its sponsoring companies.

The institute has further strengthened its academic network with other Max Planck and Fraunhofer institutes. New large-scale initiatives and research projects could be established and existing could be successfully extended such as e.g. the Max-Planck-Fraunhofer Initiative on Smart Surfaces or the Max-Planck-Fraunhofer Initiative on Polycrystal Mechanics and several initiatives with our neighbour universities RWTH Aachen (SFB 761) and Ruhr University Bochum (SFB/TR 103; Max-Planck graduate school SURMAT; Center for Electrochemical Sciences).

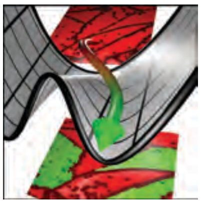
# New Research Groups



## Adaptive Structural Materials

*Theoretical group head: B. Grabowski*
*Experimental group head: C. Tasan*

Department of Computational Materials Design &
Department of Microstructure Physics and Alloy Design



A major obstacle faced in traditionally employed alloy design strategies is the inverse relation between strength and ductility. As illustrated in Fig. 1, conventional strengthening mechanisms presently employed in industrial alloy grades (blue fields) lead to a dramatic decrease in ductility. While modern advanced steels based on displacive transformations can partly break the inverse relationship (green fields), the new 'Adaptive Structural Materials' (ASM) group (initiated in May 2012) aims at developing next-generation high-strength and high-ductility metallic materials by pursuing a paradigm shift based on a novel design strategy.

The key alloy design strategy of the ASM group, intimately coupled to the SMARTMET project (see p. 25), is to **turn phase instability into material strength**. We aim at designing, synthesizing and characterizing intrinsic phase instability at the microstructural level leading to strengthening or (when necessary) relaxation mechanisms. Such mechanisms can be introduced either by incorporating dispersed phases that are close or even beyond their mechanical and thermodynamic stability limit into otherwise stable bulk alloys, or by designing the bulk material itself to be at the verge of mechanical or thermodynamic stability. In either case the newly designed phases shall gradually transform under mechanical loading into secondary phases (*e.g.*, martensite) or extended defects (*e.g.*, twin bundles).

However, determination of instability regimes of phases in complex alloy systems and control of their instability at the microstructural level are highly challenging tasks which cannot be handled by traditional experimental or theoretical techniques. In fact, such a challenging task requires state-of-the-art *ab initio* and experimental tools employed in a closely tied joint venture. The ASM group provides a special and unique infrastructure building an excellent foundation for such extraordinary endeavors. Specifically, we combine expertise from both fields as the ASM group is built from an equal number of theoreticians (presently seven) from the Computational Materials Design department and (seven) experimentalist from the Microstructure Physics and Alloy Design department. For an optimized guidance of such a close interdisciplinary collaboration two group heads are operative.

A crucial requirement for tackling the instable phases on the *ab initio* front is an accurate and efficient description of properties at finite temperatures. We have previously developed and applied a multitude of approaches for such purposes (see Fig. 2, next page). With this, we were able to resolve a serious but very common drawback of typical first-principles applications which are bound to $T = 0$ K or other approximations. A key future challenge will be the incorporation of the various methods and techniques into a single unified approach, since we

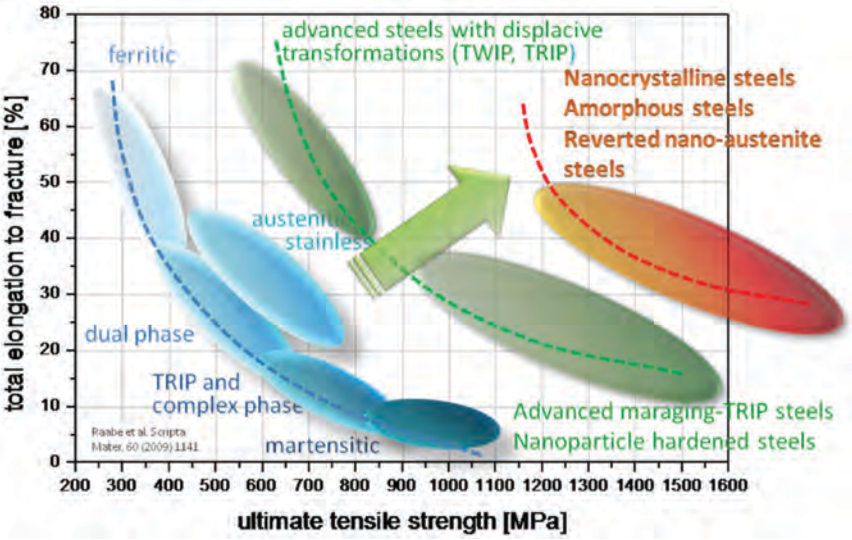


**Fig. 1:** *Inverse strength-ductility relation characterizing metallic alloys: Composition and microstructure changes make the material mechanically stronger but often reduce its ductility (elongation to failure). A major aim of the ASM group is to explore new design routes that shift the limit to the upper right part of the diagram (green arrow), i.e., that overcome this inverse relation between strength and ductility.*

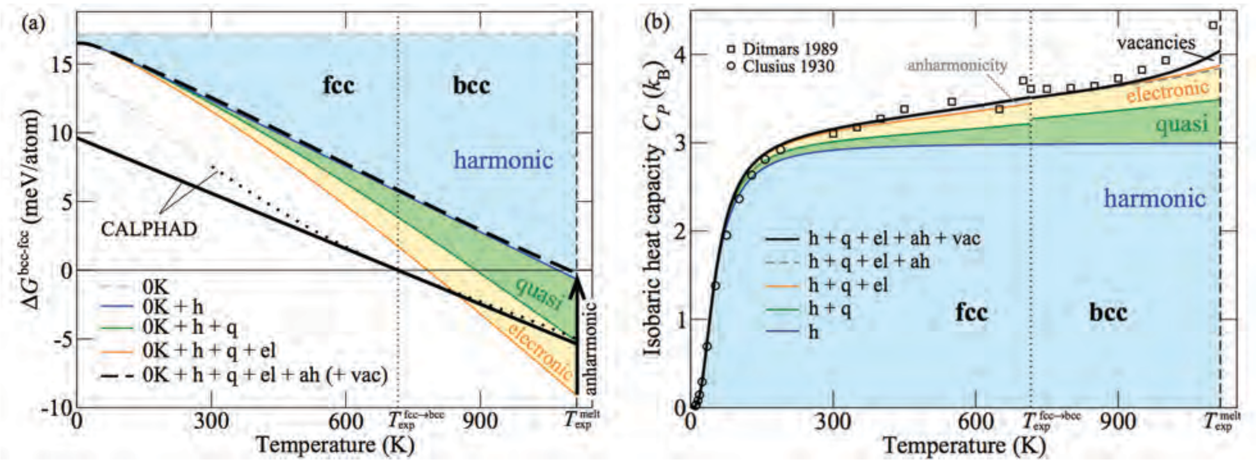


**Fig. 2.** *Importance of T>0 K contributions for the example of Ca. (a) Gibbs free energy difference between bcc and fcc. Only upon inclusion of all excitation mechanisms [(quasi)harmonic + electronic + anharmonic + vacancies] the correct T dependence is predicted (compare the slope of the dashed black line indicating full theory with the slope of the solid black line indicating experimental data). The remaining constant shift of 6 meV is focus of present investigations. (b) Heat capacity at constant pressure: again, inclusion of the various physically relevant excitation mechanisms is important for obtaining good agreement with experiment (solid black line vs. black symbols). Figures taken from Phys. Rev. B 84 (2011) 214107.*

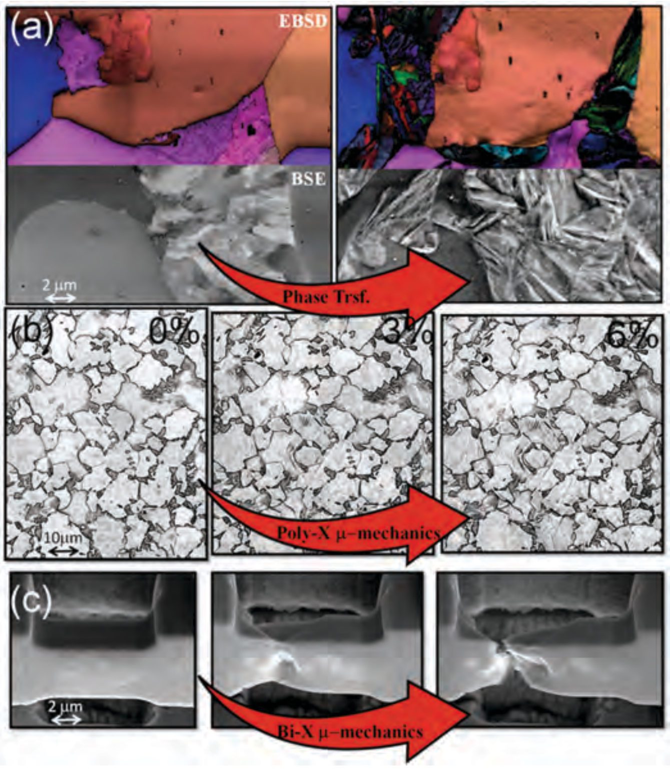


**Fig. 3:** *Results obtained using the novel experimental techniques employed in Adaptive Structural Materials group: (a) Tracking the same microstructural region through dual phase steel heat treatments: inverse pole figure and backscattered electron image of the start (pearlite-ferrite) and intercritically annealed (martensite-ferrite) states. (b) In-situ tracking of martensite-ferrite polycrystal through uniaxial tensile deformation: inverted secondary electron images taken at three deformation levels. (c) New methodology for uniaxial tensile testing of focused ion beam micro-machined microstructural regions of interest (e.g., a martensite-ferrite bicrystal, shown here): secondary electron images taken at three deformation levels.*

expect various physical mechanisms (electronic, quasiharmonic, anharmonic, magnetic, structural defects, configurational) to be crucial in the design of ASMs.

On the experimental front, we likewise rely on recently developed techniques, employing state-of-the-art microscopes that allow microstructural analysis at multiple scales. These methodologies enable tracking of phase transformations (Fig. 3a), as well as deformation micro-mechanisms in poly-/bi-/mono-crystals (Fig. 3b-c). The *in-situ* character of these techniques is of particular importance as it allows sensitive probing of stability regimes of the introduced unstable phases. Such *in-situ* analysis is strongly coupled to high (*e.g.*, atomic) resolution *post-mortem* characterization, to achieve a full analysis of relevant microstructures and also to connect to the scale at which *ab initio* simulations are carried out.

In general, it should be realized that the coupling between theory and experimentation remains challenging (even when the presented state-of-the art tools are employed) due to the typical discrepancy between **experimental complexity** and **theoretical simplification**. Our basic strategy to tackle this challenge is a controlled 'purification' of experimental conditions while systematically improving and extending the theoretical description. The 'Selected Highlight' about gum metals (p. 113) gives a specific example of this strategy.

# Combinatorial Metallurgy and Processing

## Group Head: H. Springer

Department of Microstructure Physics and Alloy Design

The mission of the group, which was established in November 2011, is to open novel pathways for the compositional and thermo-mechanical high-throughput bulk combinatorial investigation of high performance structural alloy systems. Innovative methods for the accelerated synthesis, processing and testing of bulk metallic structural materials are developed and applied, so that the associated basic metallurgical questions (e.g. alloy- and processing-sensitive changes in complex strain hardening phenomena) and corresponding engineering issues (such as texture evolution, sheet forming or joining behaviour) can be addressed more rapidly and efficiently over a wide composition and thermomechanical processing spectrum. We refer to such methods as “Rapid Alloy Prototyping” (RAP) [1]. This novel approach refers to semi-continuous high-throughput bulk casting, rolling, heat treatment and sample preparation techniques (see figure), and currently allow for the evaluation of the mechanical and basic microstructural properties of up to 50 material conditions (i.e. five different alloy compositions with ten different thermo-mechanical treatments each) within about five days. This represents a minimum time advantage of a factor of six to ten compared to established metallurgical synthesis and processing methods and step-by-step iterations of parameters. Thus the time between a design idea and the final evaluation of the materials´ mechanical and microstructural properties is reduced from several weeks or even months down to hours. Trends and critical material parameters can be reliably pre-selected, simulations verified and transient kinetic states readily investigated. This results in a rapid maturation of materials and finally the creation of “material libraries” for structural materials under full consideration of both, composition and processing. Future work aims at further increasing the screening speed, the implementation of hydrogen susceptibility and weldability in the early stages of the material design process.

Together with the ongoing developments of metallurgical and thermo-mechanical equipment for RAP and other challenging fields of metal synthesis and processing, innovative structural materials are investigated. Currently the main focus lies on austenite reversion phenomena in high strength stainless steels, the systematic investigation of lightweight Triplex steels [1], the development of high strength steels with inherent weldability (patent application pending) and methods for optimised microstructure design by the creation of local chemical gradients.

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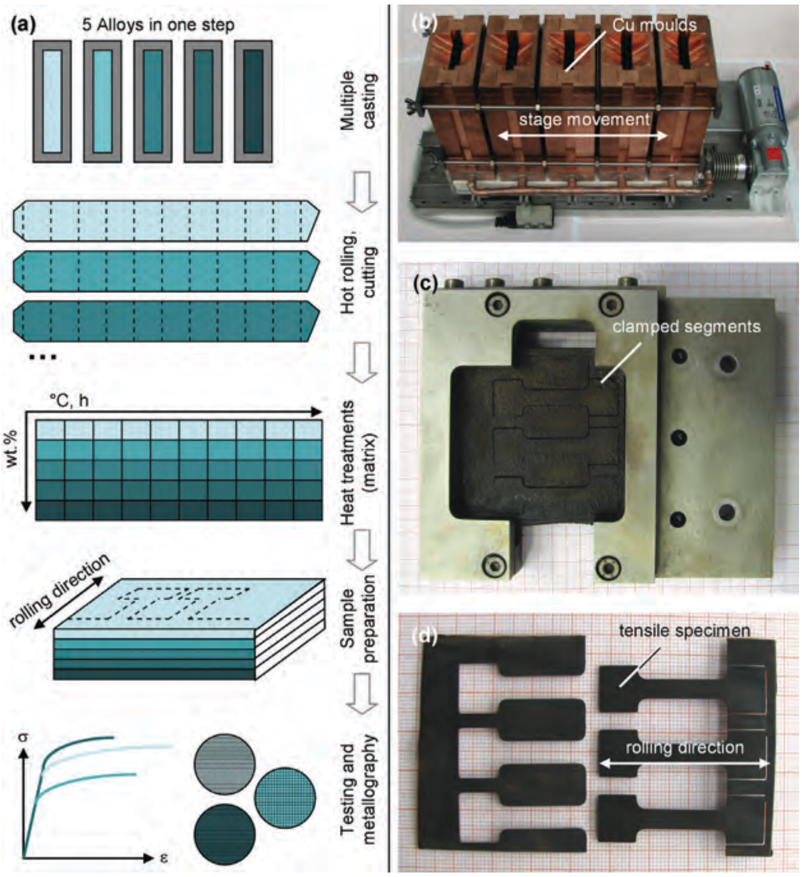

*Illustration of the sample production process for Rapid Alloy Prototyping (RAP): (a) Schematic sketch of the RAP approach where the differently shaded colours refer to the different chemical compositions, (b) device for casting five alloys into separate Cu-moulds placed on a linear stage, (c) five segments after completed heat treatment clamped together for simultaneous spark erosion, (d) one segment after completed spark erosion preparation of three tensile specimens.*

# Interaction Forces and Functional Materials

## *Group Head: M. Valtiner*

Department of Interface Chemistry and Surface Engineering

This new group was established in June 2012. The research topics in the group focus on the broad areas of adhesion, friction and interfacial forces *(i.e. Interaction Forces)*, and their organization and utilization for making new and/or better and especially energy-saving, energy efficient, cheaper, or longer lasting functional materials, interfaces and thin films for application in structural and functional materials.

The main scientific objective is to *correlate the atomic-, nano- and micro-scale properties of various surfaces, interfaces, thin films and bulk materials; their adhesion and cohesion, friction, surface degradation (damage) and wear under general environmental and corrosive conditions*. The research will in particular aim to identify fundamental physical and chemical mechanisms at the molecular, nano- and micro-scales to provide equations and scaling relations in terms of characteristic lengths, relaxation times and other properties (chemical, mechanical) of functional materials in complex (dynamically changing) environments. Materials of interest range from structural and composite materials for automotive and aerospace applications to functional/bio-motivated materials for coatings, sensing and energy applications.

Naturally, the second central focus of the group is the *design of novel experiments and experimental setups* dedicated to understanding the above described interfacial dynamics. For instance, we recently developed an approach that allows to systematically study the influence of small molecular-scale modifications of adhesion promoting bio-motivated molecules on adhesion and friction forces between apposing materials interfaces [1].

The development of novel experimental setups is centred on combining force-sensing techniques with atomic scale capabilities (scanning probe microscopies) and techniques with macromolecular as well as time-resolving capabilities (surface forces apparatus, JKR apparatus). Such combined setups will allow for the first time to mutually correlate molecular level and macroscopic properties of materials interfaces. In the figure below the newly designed electrochemical surface forces apparatus (EC-SFA), which is a central *new experimental technique available at the institute*, is described in detail. The setup developed by M. Valtiner et al. [2] allows for a simultaneous measurement of adhesion and friction forces, and absolute surface-surface separations between apposing electrified interfaces.

Future projects will focus on the direct correlation between friction forces and damage within friction traces by a combined approach of SFA (macroscale), AFM (micro- and nanoscale) and high-resolution imaging and elemental mapping techniques. Likewise, the investigation of adhesion forces and in particular the correlation of molecular recognition forces and macroscopic adhesion forces - based on *design and synthesis of adhesion promoting and structure guiding molecules* - will be a central focus of the group. Current projects and research topics of the group are listed on p. 70.

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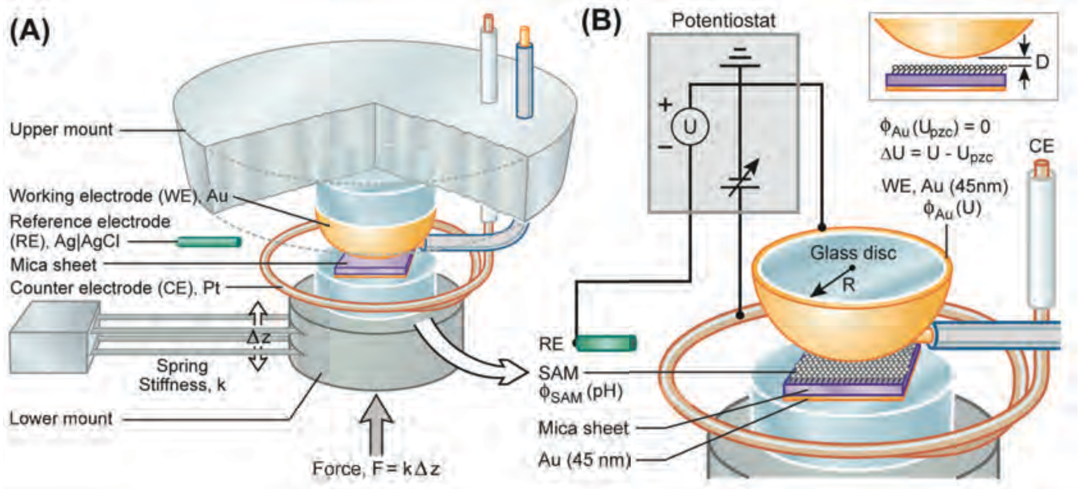
2. Valtiner, M.; Banquy, X.; Kristiansen, K.; Greene, G.W.; Israelachvili, J.N.: Langmuir 28 (2012) 13080.



*(A) Schematic of the EC-SFA. (B) Close-up of the experimental system. In this setup we apply an external electrochemical potential to an electrode (in this case Au, any metal can be used) and measure the ensuing force distance curves or friction forces due to lateral sliding. During experiments, the applied electrochemical potential U is both measured and controlled with respect to the Ag|AgCl electrode (RE).*

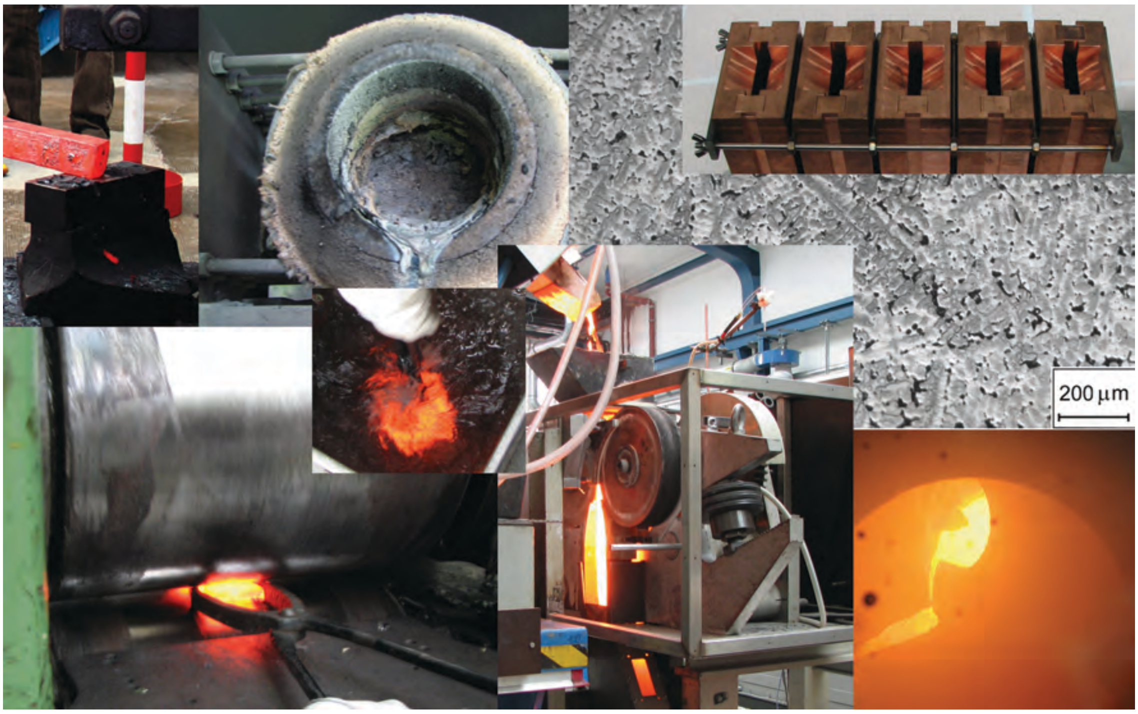
# New Scientific Laboratories and Facilities

## Metallurgy and Processing Laboratory

*H. Springer*

The new metallurgy and processing laboratory was established in November 2011. Ongoing restructuring of existing and well-proven equipments as well as the installation of new cutting edge synthesis machinery enables the production and processing of a wide range of complex metallic materials for both in-house co-operations and external scientific and industrial partners. The spectrum of materials ranges from novel lightweight metallic systems such as Gum-titanium or magnesium-based alloys with additions of rare-earth elements, intermetallic materials such as Laves phases, to amorphous alloys such as bulk metallic glasses. The main expertise, however, lies on the synthesis and processing of innovative iron based materials, for example lightweight-construction steels containing high amounts of manganese, novel creep resistant steels for energy conversion applications or high-nitrogen alloyed austenitic and ultra-high strength martensitic steels. The available instrumentation ensures maximum flexibility for a multitude of possible experimental conditions, ranging from highly controlled scientific experiments to material production close to industrial processing.

The equipment for synthesis of metallic materials comprises of several vacuum-induction furnaces (charge weight about 200 g to 70 kg under various atmospheric conditions), direct-strip-casting equipment (twin-roller setup), electron beam re-melting facility (ultra-high purification), Bridgeman-type furnace (single- and oligo crystalline materials), several arc- and levitation-melting furnaces (small charge, high purity synthesis) and rapid solidification techniques (melt spinning, liquid metal injection, splat cooling). Thermo-mechanical processing can be performed on several rolling mills (hot and cold-rolling), forging- and swaging-hammers (billet size about 100 to 5 mm) and wire-drawing equipment (down to 0.05 mm diameter). A wide selection of furnaces is available for conducting heat treatments from 50 to about 2000 °C and more under various conditions concerning atmosphere, heating media, heating- and cooling rates and sample size. A new Laser facility is currently being installed for welding, brazing, local amorphisation and other surface treatments requiring highly controlled extreme thermal kinetics.



*Snapshots from the lab: Making, shaping and treating of metallic materials*

# High-Throughput Screening for Efficient $CO_2$ Reduction Catalysts with Coupled Analysis of Reaction Products

*S. Cherevko, N. Fink, A. Zeradjanin, I. Katsounaros, K.J.J. Mayrhofer*

The (electrochemical) conversion of $CO_2$ into energy carriers like methane or methanol, as well as valuable chemicals such as ethylene, belongs to the modern "dream reactions" [1]. The fundamentals as well as the applied aspects of this reaction will be investigated in a dedicated laboratory in the Department of Interface Chemistry and Surface Engineering supported by the BMBF (ECC$O_2$, Kz: 01RC1101A). The approach, which will lead to an improvement of the understanding of the underlying processes and in consequence to the design of efficient catalyst materials, is particularly based on the development of advanced techniques coupling high-throughput electrochemistry with online product analysis [2].

The core of the main experimental setup is based on the at the institute already well-established scanning flow cell (SFC) (see figure, right), which enables the reliable execution of fast and fully automated measurements. The SFC coupled to an inductively coupled plasma mass spectrometer (ICP-MS) has already been successfully utilized in online analysis of electrode degradation products in stability tests [3]. In order to additionally analyze various volatile reaction products particularly of the complex $CO_2$ reduction directly in the product stream, we currently implement an SFC that will be operated in conjunction with a differential electrochemical mass-spectrometer (DEMS) with a membrane inlet system in the new laboratory. As a consequence, the selectivity can be determined parallel to the activity and stability, in dependence of the electrode material composition/structure and operating conditions, as well. Due to the modular construction of the whole setup, the coupling of SFC with ICP-MS and DEMS can be adjusted on demand and in future eventually also utilized in combination. Further analysis techniques like gas- and liquid chromatography will also be installed in the laboratory and used for complementary long-term electrolysis experiments.

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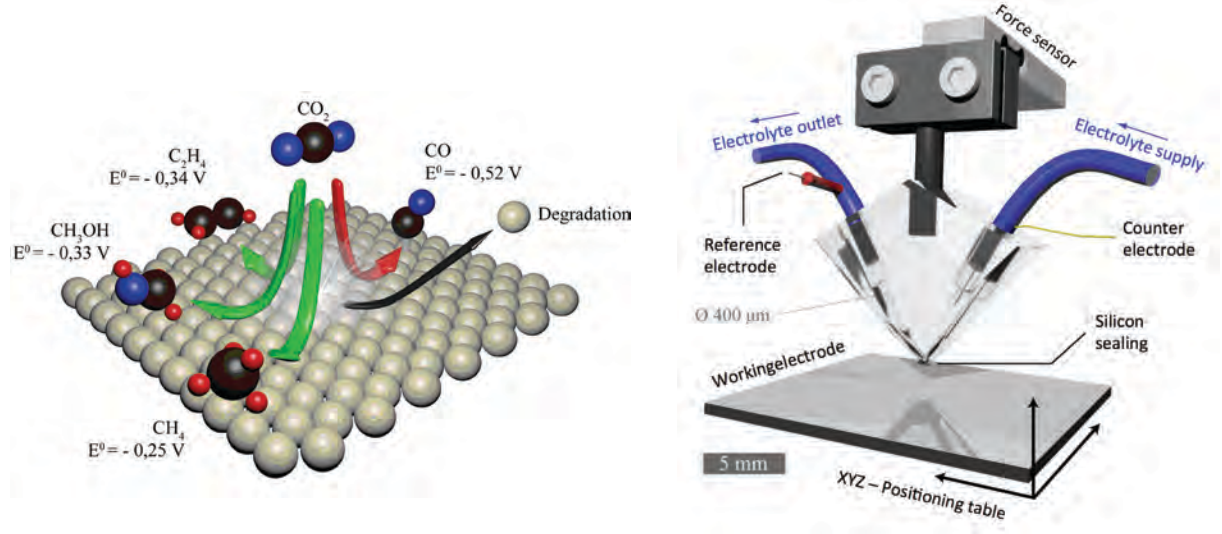


*Scheme of the possible $CO_2$ reduction products including their standard potentials (left), and the scanning flow cell used for the electrochemical high-throughput screening investigations (right) [2].*

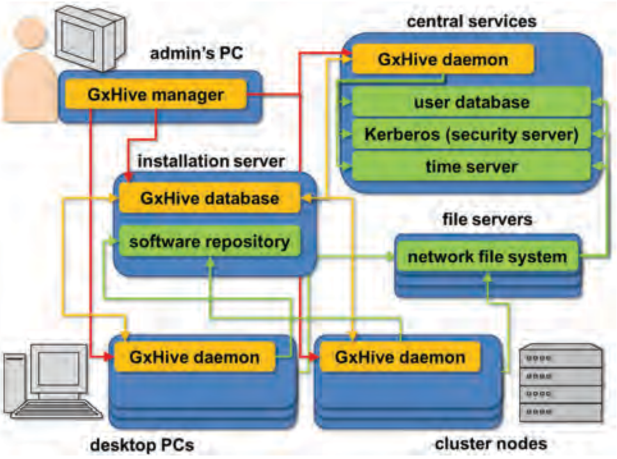
# The GxHive Cluster Administration Package

*C. Freysoldt, W. Vogt, V. Bubnik, S. Boeck*

The philosophy of the CM computer centre is - rather than offering defined services - to fulfil the needs of the computational scientists to the best possible with the available resources. For instance, we do not limit the runtime of any calculation, which not only enables arbitrarily long calculations, but also relieves the scientists of applying crude estimates in advance or sacrificing computational efficiency in favor of short runtimes. This consequent focus on the scientists' perspective makes the setup of the computer centre challenging. Specifically, the following conditions are mandatory: (1) a high availability of computational resources, (2) the unconstrained possibility to drive the hardware to its limits, (3) a high level of security to protect the confidentiality of our industrial partners, and (4) a timely response to software requests. With growing size of the department and the computer cluster - presently, our cluster encompasses almost 500 computers with about 1000 new calculations being submitted to the cluster queue every day - maintaining our standards proved increasingly difficult. To break the connection between the size of the computer centre and the administration effort, a novel administration concept was developed and implemented for us by Gemmantics IT Consulting, a spin-off company founded by the former head of the CM computer centre, Sixten Boeck.

The concept is realized in the GxHive administration software. The core idea is to store the complete setup of the CM computer centre - consisting of a 7000-core high-performance computer cluster, ~50 workstations, several fileservers, and modern network services for interoperability and security - semantically (not textually) in a database, handled by the GxHive installation server. The database is read by the GxHive daemon, a small program running on each administered computer. The GxHive daemon then downloads new software, translates the information from the database - according to rules contained in the database - into textual configuration files for the software packages installed on that computer, or runs special commands. For remote control via the network, the GxHive daemon also offers unsecure and SSL-encrypted communication channels, the GxHive ports. Administration events can be triggered by the GxHive daemon itself (e.g. at startup, or on regular intervals), by manual request via the encrypted GxHive port, or even by the GxHive installation server if it detects from the dependencies stored in the database that an administration event on a third computer (say: a software update on a fileserver) requires changes (e.g. update and restart of the client). The human administration of the computer centre consists in manipulating the database with appropriate tools. Everything else is managed by the GxHive administration package.

This approach offers a number of advantages. For instance, an individual scientist may have special software installed locally on his or her PC. This setup is mirrored in the database. If a PC hardware breaks down (which happens regularly in a department of this size), a replacement PC can be quickly set up from the database. Within an hour, the scientist can return to his usual working environment. Likewise, software updates for the cluster can be defined in the database when they become available, and can be applied with delay, e.g. when the software should not be updated while the previous version is in use. This greatly reduces collisions of administration needs with usage, and is a prerequisite for our unlimited runtimes.



*Cluster administration with GxHive uses manual (red) and automatic (yellow) communication via the GxHive protocol. System components communicate among each other and with GxHive via standard protocols (green). Blue boxes indicate separate hardware.*

This approach works nicely for software updates or full installations of our PCs. However, an upgrade of the operating system on the 500 cluster nodes or similar standardized installation tasks take a long time since the installation server has a limited throughput. To solve this issue, an image-based multi-cast installation has been developed. Here, the replication of the installation data for each node is not done by the installation server, but rather by the network switches. The database server sends out the image once, and the network switches ensure that this is copied to each individual node without any significant overhead over a single-node installation. Using this technique, the cluster can now be upgraded within 20 minutes rather than three days.

# Large-Scaled and Networking Projects

## The International Max Planck Research School for Surface and Interface Engineering in Advanced Materials:

## Second Period Is Running Successfully

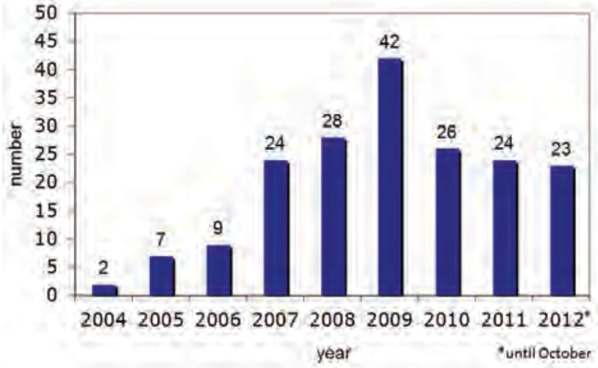
*E. Gattermann, A. Erbe*

**Introduction.** The International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS-SurMat) is a structured integrated doctoral program for gifted students. It provides excellent research conditions plus an intensive and interdisciplinary teaching experience. While most students are offered scholarships, the school is open to students funded from outside SurMat as long as all required criteria are met. The IMPRS-SurMat is a joint school of the MPIE, the Max-Planck-Institut für Kohlenforschung in Mülheim (MPIK) and the Ruhr-Universität Bochum (RUB). In addition, three Chinese universities are involved, located in Xiamen, Beijing and Shanghai. The second running period of six years started in 2010 and will end in 2015. At the moment, half of the second running period has passed, offering the chance for reflection on the past achievements and a the chance for a look ahead.

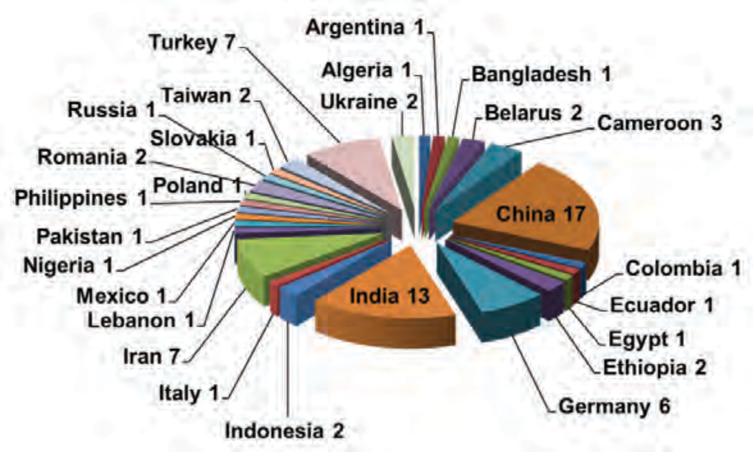
**Organization.** The SurMat board consists of five professors who decide upon the direction of the school. The two spokespersons of the IMPRS-SurMat are Martin Stratmann (MPIE) and Gunther Eggeler (RUB). The coordination of the IMPRS-SurMat is managed at the MPIE. Andreas Erbe remains scientific director, however, the former administrative director Rebekka Loschen left the institute in August 2012 and Elke Gattermann is now dealing with the administrative matters. At RUB, Christoph Somsen completes the team. He assists the students with the enrollment and is responsible for the financial management on the side of RUB.

**Students.** Towards the end of the first running period, the number of students decreased, as students finished their doctorate. With the start of the second running period, an increase in the number of students shows the re-invigoration of the IMPRS (see figure). Students are selected in two application rounds a year. From more than 500 applications from all over the world, 22 students have been selected for a scholarship. Overall, since 2010 26 new students started their doctoral work. In the second running period, the school strives to fund in total 36 students with scholarships. Overall 80 students from 27 different countries joined the IMPRS-SurMat since the beginning in 2004. Many students come from China and India; only a few are German (see figure). Since 2004, 39 students have successfully finished

Number of SurMat students.



Number of publications by SurMat students in peer reviewed journals.



*Origin of SurMat students by countries.*

their doctorate within the IMPRS-SurMat and the scientific output is very high. Besides more than 130 poster and oral presentations, 184 journal articles have been published (see figure).

**Science.** The partners of IMPRS-SurMat bring in their expertise in different areas such as metallurgy, surface chemistry, corrosion, catalysis, computational material design and atomistic modeling of interfaces. In this way, the research school covers topics ranging from fundamental scientific issues to engineering applications, both in experimental and theoretical work. Additional impulses are given by industrial partners, who sponsored four scholarships since 2010. As the students normally have two supervisors from different departments, scientific interchange and interdisciplinarity of the school are guaranteed.

**Curriculum.** The curriculum was improved, responding to student's needs. Since 2010, students have the choice to select two of four elective modules, while all have to attend four compulsory modules. Compulsory modules impart fundamental knowledge; the elective courses focus on specialized topics in selected fields. Each module consists of a one week block course. The offering of soft skills training sessions was increased in the second running period. Currently, two trainings are taking place annually. The topics focus on scientific writing, presentation skills and leadership skills. Students have to present annual reports to ensure progress of their work, with an appropriate level of supervision. After two years of working on their topic, a second year discussion is scheduled to ensure a well-planned final stage of the work. Thus, the studying times can be shortened.

**Specials events.** After a break of four years another SurMat Workshop is held in November 2012. It is a joint workshop together with the RUB‘s annual Materials Day. The workshop gives an overview of the current research topics of SurMat and the RUB‘s materials research department. Three external guest speakers from the SurMat partner universities in Xiamen and Beijing, China, have been invited.

**Outlook.** There will be three main aspects in the second half of the running period. Firstly, more new students shall be attracted to reach the level of 30 students and to award the scholarships as planned. The students who are currently in IMPRS-SurMat will be assisted to bring their doctoral work to a successful end. Preparations have already begun for the next evaluation, scheduled to take place in 2014. In particular, the scientific direction of IMPRS-SurMat has been discussed and a new concept has been worked out. The SurMat board, the directors and the SurMat community will spare no effort to make the evaluation successful so that the IMPRS-SurMat will be able to continue its fruitful work beyond the year 2015.

# Center for Electrochemical Sciences

*S. Seisel*, K.J.J. Mayrhofer, A. Auer**, A. Erbe, F. Renner,*
*W. Schuhmann*, M. Stratmann*

* Ruhr-Universität Bochum, Germany; ** Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr, Germany

As one winner of the HighTech.NRW competition the Center for Electrochemical Sciences (CES) of the Ruhr-Universität Bochum has been founded in October 2009 by the Ruhr-Universität Bochum and the Max-Planck-Institut für Eisenforschung Düsseldorf, with additional financial support by ThyssenKrupp Steel. CES is regarded as a Center of Excellence with the task to ensure international competitive research in all aspects of modern electrochemistry at the highest standard.

From the beginning on the founding members of CES, Ruhr-Universität Bochum, Analytische Chemie – Elektroanalytik & Sensorik, Max-Planck-Institut für Eisenforschung, Abteilung Grenzflächenchemie und Oberflächentechnik, and DOC Dortmunder OberflächenCentrum have intensified their collaboration. To date the CES is fully operational with a modern electrochemistry laboratory equipped with more than 15 research potentiostats including different electrochemical cells, electrochemical quartz micro balances, impedance spectroscopy, scanning electron microscopy, atomic force microscopy, surface plasmon resonance, raman spectroscopy and dynamic light scattering. The laboratory is successfully used by its members and three junior research groups. The scientific work of the last two years was focussed on a broad range of electrochemical topics including:

- improvement of the performance of lithium ion batteries through new electrode and electrolyte materials
- development of carbonaceous materials as noble metal free catalysts for the ORR
- basic understanding of electrocatalytical processes for an rational design of new catalyst materials
- experimental and theoretical understanding of thin semiconducting oxide layers
- improvement of electrontransfer processes in biofuel cell
- development of new energy conversion and storage systems like mixing entropies batteries
- nanostructured catalyst for the use in battery and fuel cell applications
- catalysts for photoelectrochemical water splitting,

To afford an experimental and theoretical work on these topics beyond the state of the art, an additional focus of CES is dedicated to the development of new analytical methods and tools e.g.:

- combination of different electrochemical methods like simultaneous cyclic voltammetry and impedance spectroscopy
- coupling electrochemical methods to other techniques like Raman spectroscopy, quartz micro balances, atomic force microscopy, surface plasmon resonance or mass spectrometry
- development of new microelectrochemical techniques which allow the use of scanning electrochemical microscopy and scanning droplet cells for high throughput measurements, for electrochemical structuring of surfaces as well as with implemented additional methods like impedance spectroscopy or photocurrent measurements.

During the last two years scientific results have been published in more than 40 papers and a number of new research projects like a BMBF-Nachwuchsgruppe for one of the junior group leaders or participation of CES in a Helmholtz-Allianz could be initiated which will lead to intense future scientific activities within CES.

Official Speakers: Prof. Dr. W. Schuhmann (RUB, Bochum), Prof. Dr. M. Stratmann (MPIE, Düsseldorf)

Scientific Coordination: PD Dr. Sabine Seisel (RUB, Bochum)

Official internet address: http://rub.de/ces/

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# Interdisciplinary Centre for Advanced Materials Simulation – ICAMS

*J. Neugebauer, T. Hickel,*
*R. Spatschek, M. Stratmann*

After five years of operation, the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) has developed to a leading institution for scale-bridging materials modeling. Due to its significant scientific output and the large variety of activities initiated by ICAMS, it has now a strong reputation in the scientific community. Not only was the MPIE a driving force in developing the idea and concept of ICAMS, it also has always been involved in its research and continues to be an integral part of the network.

The mission of ICAMS to develop, implement and apply multiscale tools for the understanding and prediction of technical materials started with the foundation in March 2007. In all years since then it was an important aspect of the work at ICAMS, to transfer the basic knowledge and the newly developed methods into industrial practice. In particular the industrial consortium consisting of ThyssenKrupp Steel Europe AG, Bayer MaterialScience AG, Salzgitter-Mannesmann Forschung GmbH, Robert Bosch GmbH, Benteler Steel/Tube Management GmbH and Bayer Technology Services GmbH, which financially supports ICAMS, benefits from these activities. Further sponsors are North Rhine-Westphalia and the European Union.

The structure of ICAMS consists, on the one hand, of three departments at the Ruhr-University Bochum, which reflect the hierarchical multiscale structure of materials: the Department Atomistic Modeling and Simulation (headed by R. Drautz), the Department Scale Bridging Thermodynamic and Kinetic Simulation (I. Steinbach), and the Department Micromechanical and Macroscopic Modeling (A. Hartmaier). These departments are, on the other hand, closely linked to three Advanced Study Groups (ASG). The ASG Modelling (director J. Neugebauer, group leader T. Hickel) is located at the MPIE and uses *ab initio* based methods to support the materials simulation of ICAMS at the lowest scale, which is dominated by electronic interactions and individual atomic processes.

The collaboration works very effectively in terms of joint projects, currently conducted on topics like magnetic free energies, multiscale simulations of H embrittlement, chemical trends for hydrogen-vacancy complexes, interface processes during martensite formation and polymer/metal interface structures and adhesion. Several informal meetings, retreats, joint workshops, and Advanced Discussions ensure a continuous exchange of ideas and data. The activities have lead to several joint conference contributions and publications. Plans for collaborations go far beyond the initial funding period of ICAMS, which ends in 2013.

**Fig. 1**: *Discussion of the group "Thermodynamic Modelling" connecting scientists of the ASG Modelling and the STKS department (I. Steinbach) during the ICAMS Scientific Retreat 2011 in Attendorn.*

**Fig. 2**: *Members of the ASG Modelling are exchanging recent results with other members of ICAMS and its industrial partners during the "Advanced Discussions" at Bochum University in April 2012.*

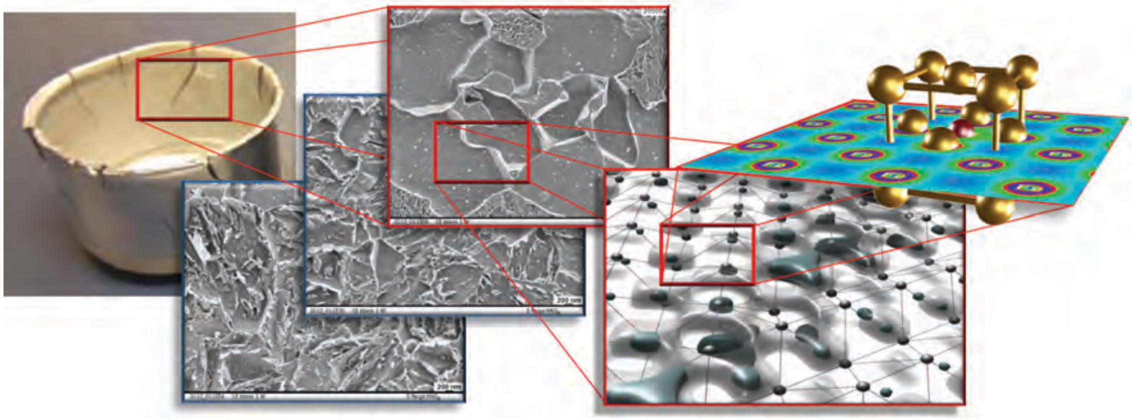
# Hydrogen Sensitivity of Different Advanced High Strength Microstructures (HYDRAMICROS): An International Research Consortium

*T. Hickel, R. Nazarov, J. Neugebauer*

The well-known problem of hydrogen embrittlement in various metals becomes increasingly important for modern advanced and ultra-high strength steels, with strength levels above 1000 MPa. Since by far not all steel grades are affected in the same way, more knowledge about the reason for deviations is needed. The importance of this topic convinced the European Research Fund for Coal & Steel (RFCS), which granted a research project on the “Hydrogen Sensitivity of Different Advanced High Strength Microstructures (HYDRAMICROS)” with more than one million Euros. The project started in July 2010 and runs for 42 months. Partners in this project are ThyssenKrupp Steel Europe AG (Germany), Onderzoekscentrum voor aanwending van staal N.V. (Belgium), voestalpine Stahl GmbH (Austria), Aalto university foundation (Finnland) and the MPIE. The coordination of this project, including negotiations with the European Commission is done by the MPIE (T. Hickel).

The premise of this research project is the understanding that a straight comparison of a variety of industrial grades with respect to hydrogen sensitivity leads typically nowhere, because of the complexity of the material: Each sample is simultaneously characterized by its own chemical composition, non-metallic inclusions, grain size distributions, phase fractions, strength levels, deformation states, dislocation densities, etc.. Therefore, the consortium aims at significantly improving the comparability of materials. The core of the scientific approach lies in the investigation of steel samples with identical chemical compositions, but different classes of strength levels (1000, 1200 and 1400 MPa) related to individual microstructures. This is achieved by performing controlled laboratory heat treatments of industrial steel samples that have experienced the same casting and rolling process. Accurate characterizations of hydrogen charged and uncharged samples before and after mechanical testing are important for assessing and ranking the material. With such an approach, the sensitivity to hydrogen embrittlement can be attributed to certain microstructure features and guidelines for further development of high-strength steels can be derived.

The MPIE and particularly the CM department provide within the consortium a theoretical understanding based on *ab initio* calculations, how single microstructure features can influence the behavior of hydrogen in the investigated steel samples. The calculations allow separation of the contribution of different phases to the hydrogen solubility and mobility from more complex structures such as phase and grain boundaries. Furthermore, non-metallic inclusions and precipitates (carbides) are considered. Even inhomogeneities (e.g. local element concentrations, grain boundary configurations, etc.) and their importance are assessed. The results are compared with experiments of the partners, which typically average over all features. An individual analysis is only possible with very sophisticated techniques (see p. 119).



*The philosophy of the HYDRAMICROS research consortium (from left to right): With the overall aim of reducing the sensitivity of a high-strength steel to hydrogen embrittlement, the influence of the microstructure is systematically studied. Different microstructures for the identical steel grade (here from the partner TKSE) are obtained by heat treatments. The ab initio simulations at the MPIE reveal the influence of microstructure features like grain boundaries and phase fractions on the behavior of hydrogen.*

# SMARTMET: Adaptive Nanostructures in Next Generation Metallic Materials

*C. Tasan & B. Grabowski, J. Neugebauer, D. Raabe*

European Research Council
Established by the European Commission

The European Research Council (ERC) rewards the most prestigious and competitive scientific funding in Europe. The sole criterion for selection is scientific excellence. In 2011, Prof. D. Raabe and Prof. J. Neugebauer were awarded an ‘ERC Advanced Research Grant’ for their pioneering project proposal: *SMARTMET: Adaptive nanostructures in next generation metallic materials*.

The objective of SMARTMET is to address the inverse strength-ductility problem, which sets an apparent limit to the mechanical strength-ductility optimization of advanced engineering alloys, by exploring new design strategies. The key idea is based on the novel strategy of designing, synthesizing and characterizing **intrinsic phase instability**. The philosophy behind that is to either incorporate dispersed phases that are close or even beyond their stability limit into otherwise stable bulk alloys or to design the bulk material itself such that it is at the verge of stability. In either case the newly designed phases shall gradually transform under mechanical loading into secondary phases (*i.e.*, martensite) or extended defects (*e.g.*, twin bundles).

Well-controlled introduction of such unstable phases enhances the overall ductility and strength of the material by inducing deformation-driven transformations in critical regions such as crack tips, which cause local strain hardening overcompensating localization and avoiding failure initiation (Fig. 1). Examples include transformation-induced plasticity, twinning-induced plasticity, bulk phase instability close to transition points, shape memory, or mechanical alloying phenomena. Using this concept we expect to turn well localized phase 'weakness' into compound 'strength' and ductility.

The SMARTMET project has a horizon of five years. Over this period, the funding covers three post docs, four Ph.D. students, and two senior scientists. The personal is split into an equal number of experimentalists and theoreticians. SMARTMET is embedded into the Adaptive Structural Materials group (p. 13) and the leadership lies in the hands of Dr. C. Tasan − an expert in *in situ* microstructural techniques − and Dr. B. Grabowski − an expert in finite temperature *ab initio* simulations. An intensive coupling between experiment and theory is the primary trade mark of the SMARTMET endeavor being essential for a successful realization of the ambitious aims.

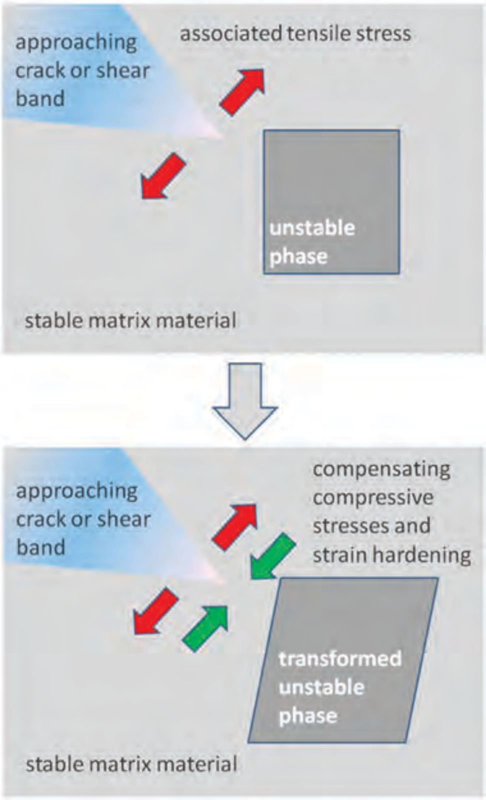


**Fig. 1:** Mechanical *response of an unstable second phase embedded in an otherwise stable matrix on an approaching load. In the schematic case depicted the transformation is associated with a volume change and shear. The resulting local stress field upon transformation of the unstable phase can stop localization and damage initiation effects.*

IDEAS
The European Union's
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ERC Advanced
Research Grant
SMARTMET

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

*F. Roters, T. Hickel, R. Spatschek, S. Sandlöbes, P. Choi, S. Zaefferer, B. Svendsen, D. Raabe, J. Neugebauer*

In 2007 the Max-Planck-Institute in Düsseldorf (MPIE) and RWTH Aachen University jointly initiated a collaborative research center (Sonderforschungsbereich, SFB 761) on the 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 first four year phase of the SFB 761 ended in June 2011. The results were successfully presented during the evaluation of the SFB in early 2011. Based on this evaluation and the written report a second four year phase was granted by the DFG.

The key idea of the SFB 761 is to develop a new set of methods for material- 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 is now extended to Fe−Mn−Al−C. This extension allows a systematic study of the transition from alloys showing the TWIP effect, which were in the focus during the first four years, to alloys showing the TRIP effect (TRIP: transformation-induced plasticity; TWIP: twinning-induced plasticity). As a second topical extension the role of hydrogen will now also be studied by use of *ab initio* and experimental methods. In the field of characterisation, new techniques, namely Atom Probe Tomography (APT) and Nuclear Magnetic Resonance (NMR) spectroscopy, are introduced into the SFB. Finally, alternative production routes based on strip casting will be studied. To cover all these new topics the SFB was extended to 22 projects in total. Six of these projects are placed at MPIE and another two are jointly run by scientists from MPIE and RWTH Aachen.

As the SFB 761 aims at developing new methods of steel design it is especially noteworthy, that with the second phase of the scientific program also the first transfer project was established. Transfer projects aim at knowledge transfer from the SFB into industry. Some of the tools developed during the first four years are in this case applied to Fe−Cr−Mn−N(−C) steels in collaboration with ThyssenKrupp Nirosta (now Inoxum).

Inspired by the success of the first period, SFB 761 will continue in the manufacturing and characterization of Fe−Mn−Al−C-steels of different compositions, the use of *ab initio* methods for the prediction of key thermodynamic parameters (relevant, e.g., for TWIP, TRIP, weight reduction, shear band formation and kappa-carbide formation), and 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.

*The SFB 761 team during the workshop in Freiberg in September 2011.*

# Cluster of Excellence RESOLV

*S. Borgmann*, A. Erbe, F. Renner,*
*M. Havenith-Newen*, M. Stratmann*

*Ruhr-Universität Bochum (RUB)

The new research field Solvation Science will be strongly enforced by the recently funded Cluster of Excellence RESOLV ("Ruhr Explores Solvation"), hosted by RUB (Speaker: Martina Havenith-Newen). The five year funding period from the DFG starts at the 1st of November 2012.

The mission of RESOLV is to launch Solvation Science as a new interdisciplinary field to understand the influence of solvation on reactions, the function of biomolecules, and processes at liquid-solid interfaces. Solvation Science will provide a unifying framework for understanding solvent processes and allowing them to be engineered in a predictive fashion, complemented by fostering the fast transfer of advances from fundamental research into industrial applications. Solvation research will find its new home on RUB campus in 2015 in the state-of-the-art research building ZEMOS (“Center for Molecular Spectroscopy and Simulation of Solvent Controlled Processes”), approved by the Wissenschaftsrat (2011).

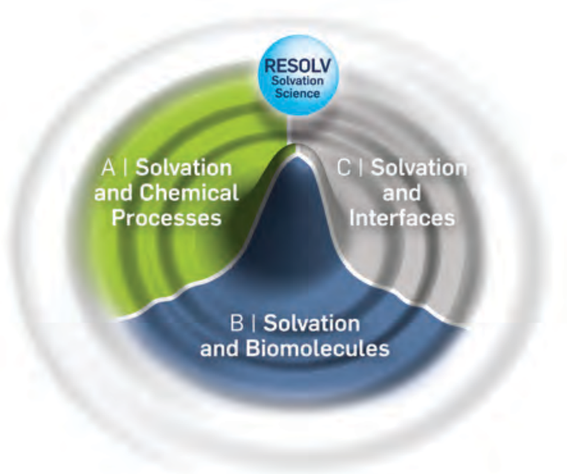
RESOLV represents a new stage in the cooperation between three universities and four leading non-university institutions in the Metropolis Ruhr: RUB, Technische Universität Dortmund, Universität Duisburg-Essen; Fraunhofer-Institut für Umwelt-Sicherheits- und Energietechnik (UMSICHT); MPI für Chemische Energieumwandlung, MPIE, and MPI für Kohlenforschung.

The research within RESOLV aims at providing a unifying framework for understanding solvent processes and allowing them to be applied in a predictive fashion. The scientific program of RESOLV is focused on three research areas:

- Research Area A: Understanding and Exploiting Solvation in Chemical Processes
- Research Area B: Connecting Solvation Dynamics with Biomolecular Function Processes
- Research Area C: Ion Solvation and Charge Transfer at Interfaces Processes

With expertise in surface preparation, surface analysis, simulation and electrochemistry, MPIE will be strongly involved in research area C. Aim of the work at MPIE will be an understanding of the role of solvents and solvation in electrochemical reactions, like oxygen reduction, oxygen evolution, metal deposition and metal dissolution. One of the early career researcher groups to be established within RESOLV will be hosted at MPIE, and will focus on the analysis of electrochemical reactions with sum frequency generation spectroscopy.

Speaker: Prof. Dr. Martina Havenith-Newen
Internet address: http://www.rub.de/solvation/



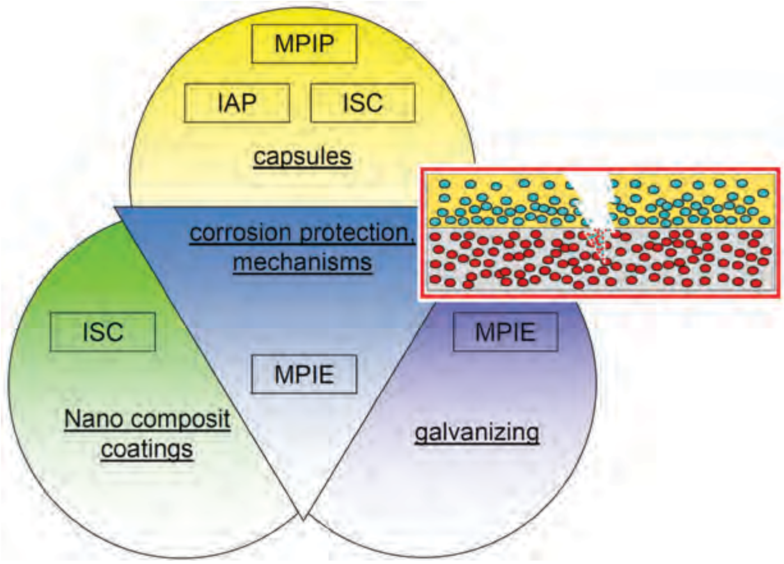
*Research areas within RESOLV ((C) Ruhr-Universität Bochum).*

## Cooperation between Max Planck Society and Fraunhofer Society:

# Active Coatings for Corrosion Protection – Aktive Schichten für den Korrosionsschutz (ASKORR)

*M. Rohwerder*

Within the framework of the research alliance between the Max-Planck-Society and the Fraunhofer Society a joint research project on active coatings for corrosion protection started in may 2010. Besides MPIE the partners in this cooperation are the Max-Planck-Institut für Polymerforschung (MPIP) in Mainz (Prof. Landfester), the Fraunhofer Institut für Silicatforschung (ISC) in Würzburg (Dr. Schottner) and the Fraunhofer Institut für Angewandte Polymerforschung (IP) in Golm (Dr. Jobmann). The expertise in this team ranges from electrochemistry and corrosion over synthesis of nano- and micro-capsules to organic-inorganic hybride coatings. The main target of this project is to develop coatings that contain self-repair agents stored inside suitable nano-capsules. Only in case of corrosive attack these capsules should release the active agents and stop the corrosion as well as repair the defect in the coating that was the cause for the corrosion. One of the main problems for achieving good self-healing is to store sufficient amounts of active agents for also closing defects larger than a pinhole. Synergy between components stored in the zinc coating and components stored in the organic or hybrid inorganic-organic coating is the approach investigated in the framework of this project. An important aspect of storing active substances inside the zinc coating is that even reactive compounds, such as catalysts for starting polymerization, will stay stable inside the zinc coating and survive even for years, as there is no contact with oxygen from the air. In the organic or hybrid inorganic-organic coating that is applied on the zinc coating, capsules containing according monomers are stored. Based on close cooperation between all partners within ASKORR, a coating system was successfully developed that indeed shows corrosion triggered intelligent self-healing where a scratch is fully overgrown by new organic coating. This system is steadily optimized with the aim of self-healing ever larger defects.



*Cooperation partners and their main working fields within the ASKORR research project.*

# Northern Alliance for Competence (Kompetenzverbund Nord, KVN) –

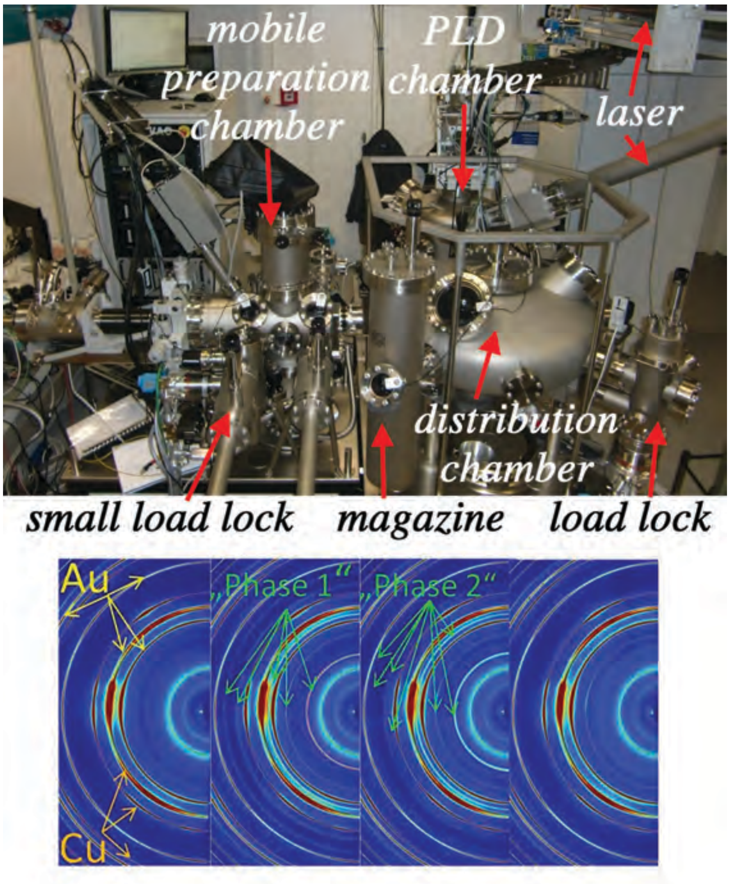
## German Research Priorities in Electrochemistry with the Focus on Electromobility:

## Studies on Model Interfaces for Li Ion Batteries

*P. Bach, A. Seemayer, N. Sathirachinda, M. Stratmann, M. Rohwerder, F.U. Renner*

There is a global need for alternative mobility schemes. Within the next decades the electrification of drives will be crucial for state-of-the-art mobility. Science needs to focus on the key technology of storage batteries in terms of high energy storage, safety and cost-efficiency. The German Federal Government's 2009 Economic Stimulus Package II included the funding of electrochemical studies with focus on electromobility. The Center for Electrochemical Studies (CES), with its partners of the Max-Planck-Institut für Eisenforschung (MPIE) and the Ruhr-Universität Bochum (RUB) contributes in this framework (KVN) with studies on model interfaces of Li ion battery anodes with a strong cooperation with its partners, the Forschungszentrum Jülich (FZJ - project leader), and the universities of Aachen (RWTH), Münster (WWUM) and Hannover (LUH). The funding period ended in June 2011.

The MPIEs activities are on fundamental questions. Especially the alloying/dealloying process of lithium into metallic anodes is investigated. For this reasons model interfaces are prepared (PLD, sputtering) and characterised with modern surface analytical equipment, such as scanning Auger microscopy (SAM), scanning Kelvin probes (SKP) and *in-situ* X-ray diffraction (XRD) employing synchrotron light facilities. The figure shows the pulsed laser deposition (PLD) system purchased for this project. It is possible to produce thin films of a range of materials which we use as model anodes for lithium ion batteries (LIB). Like nanowires or nanoporous systems they are promising to avoid problems arising from the large volume expansion of LIB anodes during Li uptake. Silicon nanowires are currently intensively investigated, because silicon has a specific capacity for Li uptake ten times higher than the still widely used graphite. For the preparation of Si-nanowires however a Au catalyst thin film is needed which influences the performance of the eventual battery. To address this we investigated the Li uptake and release of thin Au films by *in-situ* High Energy XRD (HEXRD). HEXRD is employed since it allows high penetration depth and short measuring times. The publication of first promising results is in preparation (P. Bach, A. Seemayer, U. Rütt, O. Gutowski, F.U. Renner). During Li insertion a metastable phase is formed which dissolves during Li extraction via a second metastable phase (see figure). These results will help to understand the behavior of Si-nanowires anodes during battery cycling.



*Pulsed Laser Deposition (PLD) chamber with distribution chamber, load lock and mobile preparation chamber (top). Phase formation/dissolution during electrochemical cycling of the Au thin film electrode on Cu substrate (bottom).*

# Analysis of Microstructure in Plasticity: A Joint Initiative between MPIE and Universities Bochum, Bonn, and Duisburg-Essen (DFG FG 797)

*K. Hackl*[1], *D. Raabe*[2], *S. Müller*[3], *P. Dondl*[3], *J. Schröder*[4], *D. Balzani*[4]

[1] Lehrstuhl für Allgemeine Mechanik, Ruhr-Universität Bochum
[2] Department of Microstructure Physics and Alloy Design, MPIE
[3] Hausdorff Center for Mathematics and Institute for Applied Mathematics, Universität Bonn
[4] Institut für Mechanik, Universität Duisburg-Essen

In 2008 the Max-Planck-Institute in Düsseldorf (MPIE) teamed up with a group of colleagues from Ruhr-Universität Bochum, Universität Bonn, Universität Stuttgart, Humboldt-Universität Berlin, and Universität Duisburg-Essen on the analysis and computation of microstructure in finite plasticity. The initiative is funded by the German Research Foundation (Deutsche Forschungsgemeinschaft DFG) as Forschergruppe 797. Speaker of the project is Prof. K. Hackl (Bochum). The initiative aims at a fundamental understanding of the physical origin, the mathematical behavior, and the numerical treatment of models which include microstructure with a special emphasis on patterning phenomena. This goal is pursued by mathematical analysis, numerical analysis, computational mechanics, material modelling and experiments. The mathematical analysis is based on methods from the calculus of variations, while in the numerical implementation global optimization algorithms play a central role. The modeling covers the mesoscopic length scales, from the dislocation structure up to macroscopic samples. The development of the models is compared to experiments on single- and polycrystals.

MPIE is specifically interacting with three of the projects, namely, on the experimental and theoretical investigation of deformation patterning (lamination) with P. Dondl and S. Müller; the gradual evolution of laminated microstructures with K. Hackl; and the 3D analysis of the microstructure of dual phase steels with J. Schröder and D. Balzani. The aim of the joint project is the experimental investigation of the local deformation-induced patterning of crystallographic orientations in metals and the quantitative comparison of the observed microstructures with theoretical models. As one exemplary result we report here on recent progress in uniting lamination theory and orientation patterning experiments. We quantitatively correlated the orientation patterning observed in shear deformed copper single crystals using orientation microscopy EBSD (electron back scatter diffraction) with a model of kinematically compatible laminates using a technique developed within this research initiative. The specification of the experimentally observed patterning phenomenon as a laminate the formation of which is predicted to be based on strong latent hardening is novel in the research field, see figure [1].

## References

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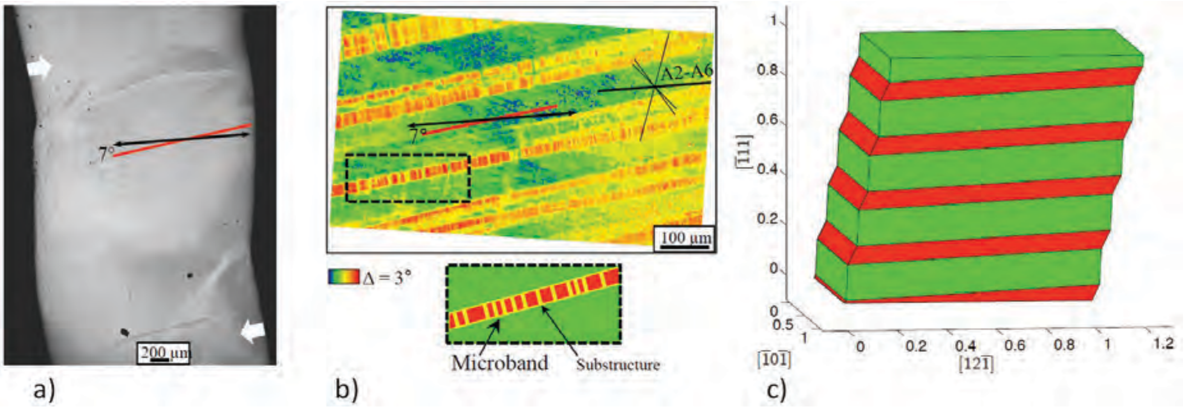


*a) SEM micrograph of a shear deformed copper single crystal. The direction of load is indicated by white arrows. b) EBSD map of a deformed area which shows the crystallographic orientation changes within 3°. Occurrence of microbands (red areas) is observed. Within the microbands, formation of a local substructure as illustrated in the inset is detected. The plane traces of the slip planes calculated from this orientation map are presented. The arrows represent the slip directions. The direction of the microbands which are tilted 7° with respect to the slip plane is indicated by red lines in both figures. c) shows the predicted deformation laminate that agrees well with the measured macroscopic strain. The green and red areas correspond to the respective areas in b).*

# Aachen Institute for Advanced Study in Computational Engineering Science – AICES

*P. Eisenlohr, M. Friák, C. Freysoldt,*
*D. Raabe, J. Neugebauer*

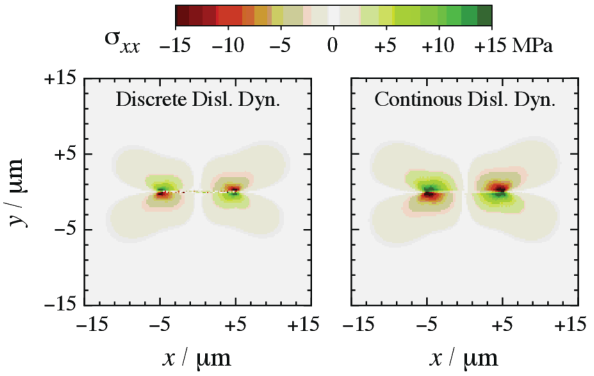
**Introduction.** The Aachen Institute for Advanced Study in Computational Engineering Science (AICES) is a graduate school that has been established within the framework of the Excellence Initiative of the German federal and state governments in 2006. In 2012 AICES was successful in securing funding from the second round of the Excellence Initiative for a period of additional five years. The Max-Planck-Institut für Eisenforschung GmbH is, together with the Research Centre Jülich, the leading academic partner of RWTH Aachen in this initiative (for details see [1]).

Dr. P. Eisenlohr (MA department of Prof. D. Raabe) and Dr. M. Friák (CM department of Prof. J. Neugebauer) became junior research group leaders associated with the AICES program during 2007. Dr. C. Freysoldt (CM) became an AICES associated young researcher in 2012.

**Mission.** The AICES program is designed to provide a thorough training at the interface of classical engineering, materials science, applied mathematics, and computer science. The focal issues are interdisciplinary inverse problems in engineering sciences, arising from increased system complexity and multiscale/multiphysics questions for which objective optimizations are sought. The AICES Graduate School complements and enhances the existing research activities at both RWTH Aachen and MPIE.

**Research topics.** Dr. Friák has been since April 2012 co-supervising the PhD thesis “Direct and inverse theory-guided combinatorial materials design of ductile Mg-based alloys employing *ab initio* and atomistic methods” of Ing. Zongrui Pei, presently enrolled at AICES and continuing from his master thesis also supervised by Dr. Friák (see [2]). The ultimate goal is to identify new alloying elements that ductilize Mg alloys by obtaining a detailed understanding of the electronic and atomistic mechanisms causing increased ductility in these industrially important materials. The study is performed in close connection with experimental investigations of Mg-alloys at MPIE (co-supervision by Dr. S. Sandlöbes, Prof. D. Raabe, and Prof. J. Neugebauer from MPIE, and Prof. B. Svendsen from RWTH Aachen).

Dr. Eisenlohr’s research activities in connection with AICES deal mostly with the micromechanics of polycrystals where the transport of lattice dislocations is influenced by the presence of grain boundaries. In the last two years, a combined finite volume/finite element approach has been developed to simulate such phenomena. We could already demonstrate that (i) size effects in crystal deformation are predominantly connected to scarcity of dislocations that carry the plasticity, and (ii) long-range internal stresses from heterogeneous dislocation distributions can be directly calculated through the elasto-plastic incompatibility *instead of* spatially integrating individual dislocation stress fields.



*Long-range stress of dislocation pile-ups at left and right ends of plastic inclusion (between -5 and +5 µm) in elastic matrix. Left: spatial integration of dislocation stress fields; right: internal stress directly resulting from elasto-plastically coupled deformation simulation.*

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1. http://www.aices.rwth-aachen.de/
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# *Ab initio* Description of Iron and Steel (ADIS): An International Workshop Series

*T. Hickel, C. Race, M. Friák, J. Neugebauer*

In 2006 the CM-department started a series of international scientific workshops on the topic “*Ab initio* Description of Iron and Steel (ADIS)”. The aim of this series is to create a platform for leading experts in *ab initio* metals research to discuss and exchange recent results and scientific developments. Such a forum is needed, because the complexity of realistic iron-based materials with respect to chemical, magnetic and micro-structure is a challenge for every *ab initio* approach, presenting no single well-paved road for simulations. Instead – to have success – a wide array of approaches and algorithms needs to be developed, implemented, evaluated, and carefully checked with respect to their predictive power. This challenge, which is well appreciated in the materials science community, can only be tackled in a combined multi-disciplinary effort.

To best fit these needs, the ADIS workshops are characterized by Gordon style, tutorial-like one hour talks, intensive discussions and, last but not least, the inspiring cooperation-promoting atmosphere of Ringberg castle (the conference centre of the Max-Planck society at lake Tegernsee). Although the *ab initio* description of iron and steel remains the main goal, each of these events has its own focus on a specific topic: The workshop ADIS2006 was called “Status and future challenges”. The focus of ADIS2008 was on approaches to the complex “Magnetism” of iron-based materials. At the ADIS2010 meeting the “Mechanical properties” of steels and related alloys were discussed.

The last meeting of this series, the ADIS2012 workshop taking place April 29 to May 04, 2012, was devoted to “Thermodynamics and Kinetics”. It addressed the fact that inclusion of temperature into *ab initio* based simulations is a non-trivial task. Only recently has a variety of computational tools been developed at the MPIE and elsewhere, to improve the capability and accuracy of *ab initio* methods in determining thermodynamic properties. Besides this, the workshop covered several techniques beyond transition state theory, for performing accurate kinetic simulations at finite temperatures. It was a further important aspect of the workshop to provide a link to the Calphad approach, since this method is of tremendous importance for the thermodynamic modeling of multicomponent materials such as steels.

The ADIS2012 workshop was the second one, to be organized together with ICAMS (namely R. Drautz), due to the common interests in the field. Furthermore, the workshop benefitted greatly from the support of the SFB761 “Stahl - *ab initio*”, in which the *ab initio* based thermodynamics of high-Mn steels is a central topic.

*56 scientists (including 15 invited speakers) participated at ADIS2012, the fourth workshop of a series on “Ab initio description of iron and steel” taking place every second year at Ringberg castle.*

# PART II.

# THE DEPARTMENTS

(in alphabetical order)

# Department of Computational Materials Design

*J. Neugebauer*

## Scientific Concept

The objective of the department is the development and application of **computationally efficient yet accurate multi-scale techniques** that are able to link the predictive power of *ab initio* approaches to the macroscopic scale, as relevant for designing and understanding structural materials for engineering applications. With increasing structural and chemical complexity of next generation steel grades the availability of theoretical/computational tools to perform all major steps in the design, analysis, or identification of synthesize routes will become more and more decisive. Only then the desired targets with respect to mechanical behavior, thermodynamic and mechanic stability or resistance against aging, corrosion or failure can be achieved.

Since the department became operational in summer 2005 it started a number of activities in that direction. One branch of activities, headed by T. Hickel, was the development of numerical tools that allow an **extremely accurate determination of all free energy contributions** by *ab initio* techniques, i.e., without having to rely on experimental input or fitting data [1]. Being able to compute highly accurate free energies opens the door to compute materials properties or kinetic processes solely on the computer. While initially applications were limited to simple bulk systems (such as non-magnetic fcc metals) enormous methodological progress allows the department now to apply these methods to real-world highly complex materials such as TWIP or TRIP steels. The methods have reached a maturity and accuracy that rival and often exceed calorimetric measurements [2,3]. Achieving *ab initio* error bars that are below the experimental ones is quite unique in solid state physics. The precision, achieved by our methods, has been successfully used e.g. to assess experimental data entering thermodynamic CALPHAD-based databases.

Another major achievement, pushed forward in the group of M. Friák, was the development of approximative but fast multi-scale methods that allow a **quick screening of materials properties**. These scale-bridging methods which connect DFT with various homogenization approaches or Ashby concepts proved highly successful in identifying optimum chemical alloy compositions, e.g., to tailor elastic properties, in uncovering hidden rules and limitations of alloys [4], or in guiding experiments e.g. in the MA department to minimize the number of samples that need to be synthesized [5]. Both approaches – extreme accuracy and fast screening – started with the initiation of the department. While in the beginning both were developed separately, the massive methodological progress achieved over the last years allows more and more often to use a combination of both and to tackle challenging materials science problems, which would be out of reach when applying a single method only.

Further cornerstones of the department, again from the very beginning, are the operation of a **high-performance computer cluster** and our in-house developed **multiscale library SPHInX** [6,7]. The 2011 newly installed computer cluster consists of 5500 cores and was ranked like its predecessor in the international Top-500 list of supercomputers. To maximize computer resources, great care has been devoted to optimize the software and to adopt it to our specific needs (see also p. 19). Both the computer cluster as well as the development of the SPHInX library are coordinated by C. Freysoldt.

C. Freysoldt is also head of the group “Defect Chemistry and Spectroscopy” devoted to non-metallic systems such as e.g. oxides. Oxides play a crucial role on steel surfaces and are fundamental to understand corrosion or coatings. Due to the existence of an electronic bandgap an accurate treatment of these materials requires to go beyond approaches that work well for metals. The group is therefore highly active and internationally well known for its method development [8]. Together with M. Todorova, who heads several projects on surfaces and electrochemistry, the group provides a strong link to the experimental and theoretical activities on oxide surfaces, electrochemistry and corrosion in the GO department.

Newly established groups complement the expertise of the existing activities. In 2010 the department was successful in appointing R. Spatschek as head of the group “Mesoscale Simulation”. In the last two years the group has been highly successful in connecting to the existing in- and out of house activities and in establishing a strong research program. For example, within the Sfb “Steel - *ab initio*” (see p. 26) the group was able to transfer the concept of an attractive H-H interaction, which is crucial to understand H-embrittlement, from the atomistic to the continuum scale in an almost lossless approach, i.e., without having to make sacrifices in the accuracy [9]. This allowed to derive complete phase diagrams, which would not have been computationally affordable if only atomistic methods were used.

Very recently (April 2012), the department has attracted B. Grabowski from the Lawrence Livermore National Lab in the US as head of the new group “Adaptive Structural Materials”. The group is financed by an ERC grant awarded to D. Raabe and J. Neugebauer and has a unique structure: It is a joint *ab initio* and experimental group and headed by an experimentalist (C. Tasan) and a theoretician (B. Grabowski). The main aim of the group is to develop concepts of how originally unstable phases may be used to synthesize smart structural materials with a microstructure that dynamically adapts to external loads. This adaptivity can be used to design mechanically superior alloys as shown e.g. for TWIP/TRIP steels.

In the reporting period there had been also changes in the group structure. A. Dick, who headed the group “Precipitation and Kinetics”, got an attractive offer as vice president at an institute of the National Academy of Sciences of Belarus and left the institute. L. Lymperakis, head of the Microstructure group for several years, received a prestigious EC grant to build up a research group in his home country at the University of Thessaloniki. He stays in close contact with the department and institute and supervises a number of projects (see p. 48). J. von Pezold, who followed L. Lymperakis as head of the “Microstructure” group, had to leave the department for family reasons. The majority of the projects initiated and supervised by him have been transferred to the group of B. Grabowski, where they ideally fit due the group’s strong focus on microstructure.

While each of the groups in the department has a high individual visibility, specific expertise and methods, the complementary character of the methods provides many successful opportunities for collaborations and resulted in several granted projects and scientific breakthroughs. Examples are the work on H-embrittlement, where three groups are involved (Hickel, Pezold/Grabowski, Spatschek) or on point defects where unique insight could be obtained by combining the metal and semiconductor community (Hickel, Grabowski, Freysoldt) [8]. Another major group bridging activity is the development of a Python-based library that automates time consuming and error prone tasks such as constructing input files for high-throughput calculations, job submission, collection of input and output data in unified databases and analyzing and visualizing the often huge output data files. The library is highly adaptive and allows to easily incorporate existing software tools such as e.g. the department’s 3D-lab which enables interactive exploration of complex crystal structures, phase transitions or defects (Aydin, Hüter, Witt, Hickel, Spatschek). The library provides also an excellent basis to build stand-alone software tools for specific materials science modeling tasks. An example is the SC-EMA tool (see Fig. 8) that provides a graphical user interface and all algorithms to compute the elastic moduli of polycrystalline materials from *ab initio* single crystalline elastic tensors (Titrian, Aydin, Friák).

The collaboration with ICAMS in Bochum has been further intensified resulting in joint publications (e.g. on the topic of H-embrittlement; [10]), conference contributions and conference symposia (e.g. a symposium on Thermodynamics at the Multiscale Materials Conference 2012 in Singapore with I. Steinbach, a symposium on Modeling Mechanical Properties with A. Hartmeier, or ADIS 2010 and 2012 and a DPG symposium 2013 on High-Throughput Methods with R. Drautz). Several members of the department (Hickel, Lange, Neugebauer, Spatschek) actively support the newly established ICAMS master course “Materials Science and Simulations (MSS)” at the Ruhr-University Bochum by giving courses e.g. on quantum mechanics, thermodynamics and statistical physics, or implementing *ab initio* techniques.

The maturity in the theoretical/computational methods achieved by the department groups provides a solid basis for joint activities with experimental groups in house and with industrial partners. The predictive power of these methods not only allows to explain/interpret experimental observations but has reached a new level allowing to make specific predictions regarding compositions or mechanisms that can be verified by experiment. Weekly joint meetings between members of the MA and CM department on various focus topics and dynamic collaborations between groups and members of the departments provide an ideal basis to combine “hot” experimental/technological questions with newest theoretical concepts. These collaborations work very successfully and several examples are given in the highlight articles (p. 101, 105, 107, 111, 113) and joint publications [4-5, 11-16].

A major aim of the department is to bring together the engineering and physics/chemistry community in the field of structural materials and to raise awareness about the specific challenges and developments. Members of the department have been therefore actively involved in organizing workshops, conferences or symposia in both communities (see p. 166). For example, our conference series “*Ab initio* description

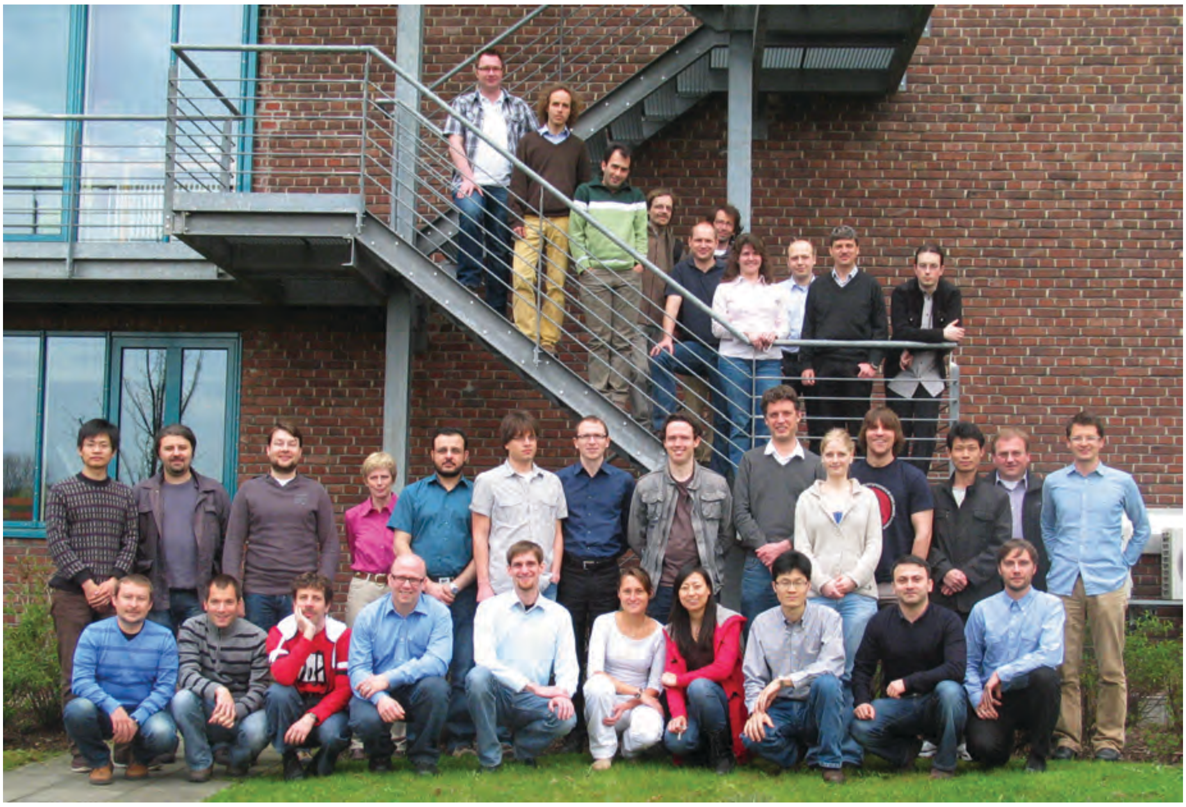


**Fig. 1:** *The CM department (summer 2011).*

of iron and steel (ADIS)" is the leading one on this topic and attracts always the top experts from both communities. The latest one, taking place in April/May 2012 at Ringberg Castle (Tegernsee), had a specific focus on most recent developments and successes in modeling thermodynamic and kinetic aspects in steels. Another example are symposia organized by the department at the German Physical Society meeting on steel and multiscale topics that show the enormous theoretical challenges in describing physically and structurally complex systems such as steel and that help to interest and recruit physicists in these topics. Related to these activities the head of the department (J. Neugebauer) has been elected as chair of the division "Metals and Materials" for the years 2013-2016.

Due to the high visibility of the scientific work members of the department received a large number of invited talks at the major conferences in the field, such as TMS, MRS, MMM, Calphad, DPG. The high scientific standards provided also the basis for successfully extending e.g. the joint RWTH-Aachen-MPIE SFB "Steel – *ab initio*" and acquiring prestigious research grants such as the above mentioned ERC grant, as well as many other national (DFG, BMBF, AvH) and European grants. Members of the group received also prestigious prizes. For example, F. Körmann received the Otto-Hahn medal of the Max-Planck society for his outstanding PhD thesis on the *ab initio* thermodynamics of magnetic systems. C. Race received an esteemed research grant from the Humboldt foundation for his highly original proposal on grain boundary kinetics.

In the last couple of years the department has grown substantially, from originally about 10 to now more than 40 members. To provide an infrastructure that connects the often very different scientific activities, the department organizes several regular weekly seminars, department retreats and social events. This allows each scientist to get an overview of all existing activities, the available and newly developed approaches and to identify contact partners for collaborations. At the department retreats, which are organized once a year, every student and scientist gets the opportunity to present results and to discuss them with members of the department as well as with our collaborators at ICAMS and other universities who traditionally join these meetings. Members of the department have been also very active in supporting the institute and its activities in the public. For example, T. Hickel scientifically coordinated the activities of the department at the ThyssenKrupp Ideenpark (see Fig. 2), a two week event where the public and specifically children are provided a hands-on experience on what makes materials science so exciting and important in modern society.

In the following the activities of the department groups and of selected project groups are briefly summarized.

**Fig. 2:** *Together with the RWTH Aachen, the MPIE demonstrated at the ThyssenKrupp-Ideenpark the concepts of a tailored materials design. 3D computer simulations (here explained by B. Grabowski, background) have been combined with basic knowledge on crystal structures and mechanical loading experiments (here demonstrated by T. Hickel (left) and C. Hüter (center)).*

## Scientific Groups

### Computational Phase Studies (T. Hickel)

The group Computational Phase Studies (CPS) is devoted to the physics of (meta)stable thermodynamic phases in metals as well as transitions between them. It is since 2006 part of the CM department. Its major vision is the *ab initio* based prediction of thermodynamic bulk phase diagrams, being directly related to many technologically relevant properties and processes in metals. The scientific performance of the group over the last two years is probably best described by the triad of ***continuity***, ***consolidation*** and ***change***:

The overall scientific scope of the CPS group is the ***continuation*** of the activities and directions established in the previous years. In the last two years the group pushed the full *ab initio* derivation of thermodynamic properties forward, using mainly density functional theory (DFT) with the aim to achieve a high precision for all relevant entropy contributions. A major focus of the group has been and continues to be on the fields **magnetic excitations**, **extended and point defects** and **hydrogen**. The following summaries (as well as some of the scientific highlights) demonstrate the substantial progress in these fields regarding the development of new methods and the derivation of new insights. As a result also the third party funding for all key projects of the group has been extended after successful evaluations.

The treatment of **magnetic excitations** within the scope of phase studies is still of central interest, since its complexity and numerical challenge makes straight-forward solutions often impossible. It turns out that even well above room temperature it is essential to take the spin quantization into account in order to obtain reliable heat capacities of materials (Fig. 3). By the development of various new techniques spin quantum Monte-Carlo simulations, originally restricted to simple model Hamiltonians, could be generalized to allow for the treatment of realistic spin Hamiltonians (F. Körmann). Using our newly developed approaches it has been possible to achieve impressive agreements of the thermodynamic properties of all unary metals [18] and compounds [2] with experiments, where in particular for chromium new insights on its magnetic behavior became apparent (see p. 149) [19]. Another important issue is the development of methods for the influence of magnetic excitations on other thermodynamic properties such as lattice vibrations. As demonstrated for Fe (F. Körmann), it now became possible to perform phonon calculations even for the challenging case of paramagnetic disorder (see p. 143) [20]. Several of these activities are performed in close collaboration with ICAMS and its CALPHAD group (S. Fries).

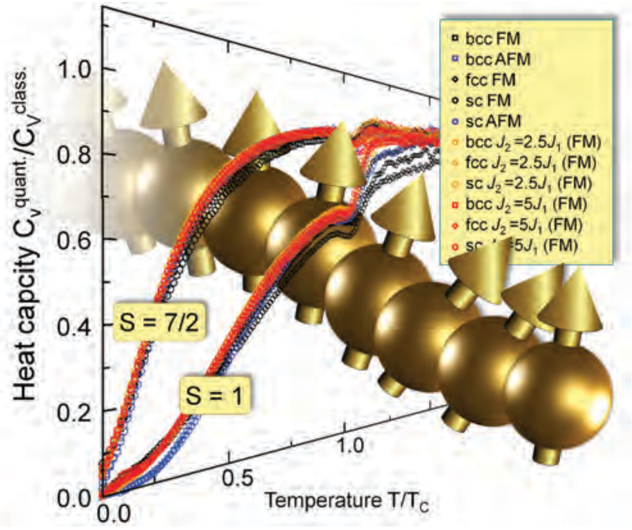


**Fig. 3**: *To compute thermodynamic properties of magnetic materials, it is decisive to take the quantum nature of spins into account. The figure shows the ratio of the heat capacities obtained from quantum vs. classical Monte-Carlo simulations for two different spins S. For a large variety of configurations, this ratio shows remarkably universal temperature dependences. For details see Ref. [17].*

Vacancies are the most prominent **point defects** in metals, due to their impact on thermodynamic as well as kinetic properties. Nevertheless, discrepancies in the vacancy formation energy between DFT and experiment made method developments decisive. This includes a correction scheme to tackle errors in the exchange-correlation functional (R. Nazarov) [21] and a breakthrough in understanding the temperature dependence of the anharmonic contribution to vacancy free energies of formation (A. Glensk, see p. 147) [22]. These activities are performed in cooperation with the ASM group and are part of a research package (PAK 461) on the thermodynamics of Al−Mg−Si−Cu alloys, which has benefited from our *ab initio* input [23] and has recently been successfully evaluated for an extension by another two years.

The thermodynamics of **extended defects** is also considered in the CPS group, mainly focusing on the stacking fault energy (SFE) (see Fig. 4). This energy determines the probability of deformation mechanisms in structural materials. The *ab initio* calculations of the dependence of the SFE on the C content [24] allowed highly interesting predictions on nano-diffusion during SFE measurements and deformations (see p. 105) [16]. In addition the influence of Al or Si [25] and magnetism (I. Bleskov) on the SFE has been studied. These and other *ab initio* results have contributed to the understanding of mechanical properties of high-Mn steels [15] and to the success of the collaborative research center SFB 761 “Stahl - *ab initio*” and its extension by another funding period starting in 2011. Precipitates form another class of extended defects, which are investigated in the CPS group. The focus in the group is on the thermodynamic stability of these phases (see e.g. p. 101), their relevance for the overall mechanical properties of the materials (in cooperation with the *Ab initio* Thermodynamics group) and the kinetics of the formation process (N. Tillack, N. Sandschneider). The influence of interfaces and grain boundaries was in the CPS group so far mainly studied in the context of hydrogen migration (see Fig. 5 and p. 119) [10].

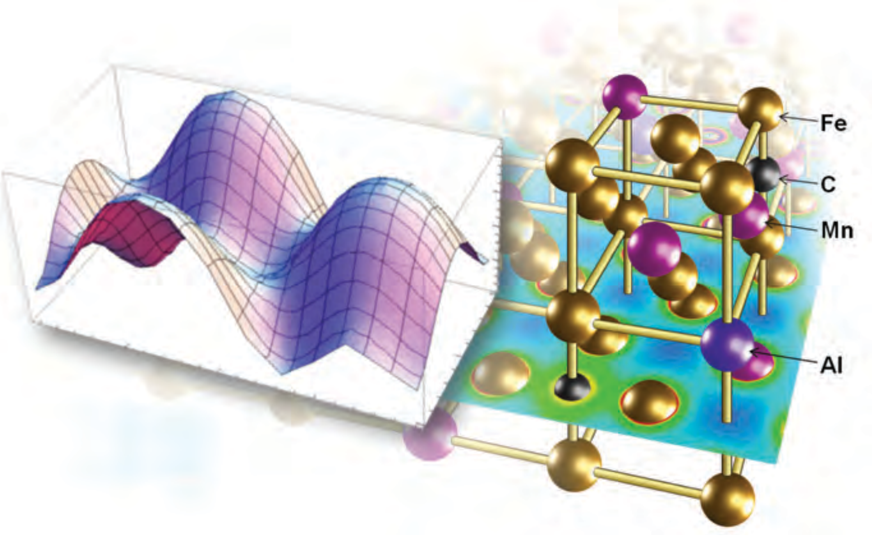


**Fig. 4:** *A major research topic of the CPS group are high-Mn austenitic steels, typically containing up to 20-25 wt.% Mn and a substantial amount of C. To reduce the embrittling effect of H, Al is often added in addition. The deformation behaviour of these materials is determined by the (generalized) stacking fault energy (shown in the inset for non-magnetic fcc Fe). Chemical as well as magnetic trends for the SFE have been systematically studied.*

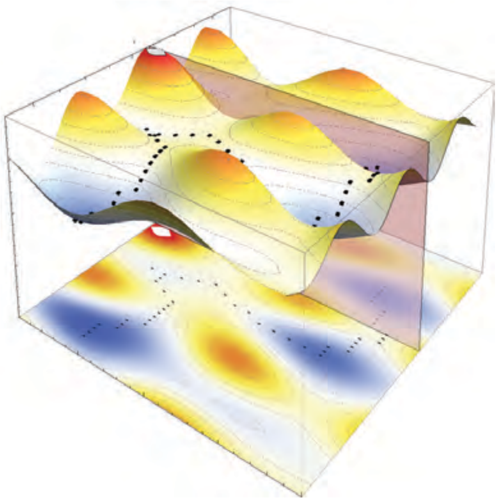


**Fig. 5:** *The interaction of H with planar defects is important for H embrittlement. This figure visualizes a possible diffusion path of H perpendicular to a twin boundary in fcc Fe. The calculations reveal a slight repulsion of the H atom from the defect***.** *For details see Ref. [10].*

**Hydrogen** is relevant for the mechanics of many materials, since it can significantly contribute to embrittlement. The CPS group (U. Aydin, R. Nazarov) therefore made intensive and systematic investigations on the solubility and diffusion of hydrogen in metals [26], including also the effect of superabundant vacancy formation due to hydrogen [27,28]. These activities resulted in an RFCS project on the relation between microstructure and hydrogen embrittlement, coordinated by the head of the group (T. Hickel). In particular the role of hydrogen in advanced high-strength steels is investigated within industrial projects (P. Dey) and the SFB 761 "Stahl - *ab initio*" (A. Chakrabarty). The research benefits from close links to the ASM group, where methods to treat the H-dislocation interaction are developed and the Mesoscale Simulation group, allowing a connection to the continuum scale.

The ***consolidation*** of the above mentioned activities in the last couple of years resulted in several review articles. The first one was devoted to free energies of point defects [29], a topic which later entered into an extended article on the *ab initio* treatment of defects [8]. Second, a highlight article in the $\Psi_k$ newsletter summarized the developed methods to obtain *ab initio* free energies of bulk phases [1]. A third review describes recent successes in the *ab initio* derivation of phase diagrams using the example of shape memory alloys [30]. The group participated in other reviews on elastic constants [4], semiconductor nanostructures [31], and hydrogen in steels.

All together, the power of the developed set of thermodynamic methods as well as their relevance for materials design are meanwhile accepted well beyond the DFT community. The above mentioned list of key research activities (magnetism, defects, hydrogen) is particularly decisive for **advanced high-strength steels,** being the reason for several joint research activities with the MA department, but also with partners in other (research and industrial) institutes world-wide. The significant contribution to the understanding and development is not only limited to structural, but applies in a very similar way to **functional materials**. Our long-standing activity in the field of shape-memory alloys, including the prediction of phase diagrams [30,32], has now been extended to their magneto-caloric properties. To perform this work we successfully applied for funding within the priority program SPP 1599 on "Magnetic Cooling". Furthermore, the links to the **CALPHAD community** are becoming more and more tight. This goes along with an increasing number of examples, which show smaller error bars of *ab initio* derived thermodynamic quantities compared to the scatter in the experimental data. One of the most recent results has been obtained for Ca (B. Grabowski), for which a complete and careful evaluation of all excitation mechanisms and in particular of anharmonic lattice vibrations revealed that a correction of CALPHAD databases is necessary [3]. Due to this kind of developments the head of the group (T. Hickel) is organizing a Calphad Unary Workshop in March 2013 in conjunction with S. Fries (ICAMS).

There have been several ***changes*** in the personnel structure of the group over the last couple of years. With A. Dick and B. Grabowski two experienced postdocs and driving forces for the research have left the group and became themselves heads of research groups in the CM department. Two other group members have gained so much experience over the last years that they are now taking over more responsibilities in the group: (i) R. Nazarov is becoming continuously more involved in the coordination of all hydrogen-related projects in the group. (ii) F. Körmann, after defending his PhD thesis excellently in 2011, is heading several research projects on magnetic properties of materials.

Two of the PhD students are also taking over responsibilities for the department. (iii) U. Aydin has started with the development of databases and is supervising the colleagues working on a joint (Python based) program package for this purpose. (iv) A. Glensk assists all interested members of the CM department in performing phonon calculations. Other colleagues have recently joined the team: (v) I. Bleskov is now performing the research within the SFB761 and is also responsible for introducing CPA-EMTO methods to the group. (vi) B. Dutta works on magneto-caloric materials and will introduce new methods to calculate phonons for chemically disordered alloys. (vii) X. Zhang will study martensite formation as a Surmat PhD student. (viii) P. Dey strongly supports our understanding of H in high-Mn steels. Finally, there is an ongoing collaboration with O. Marquardt on applications of the $k \cdot p$ formalism [33,34].

### *Ab initio* Thermodynamics (M. Friák)

The group aims at identifying **multi-scale structure-property relations** and uses theoretical methods to identify fundamental mechanisms governing the behavior of materials. The prime motivation is to use scale-bridging concepts (see e.g. Fig. 6) in a theory-guided materials design of new alloys that allows adapting in a fast and flexible way to the often dynamically-changing industrial needs. The **ductility of materials, their strength, and the identification of alternative solutes** are among the key objectives of the group. In order to properly address them, physics-based theoretical methods are combined with engineering phenomenological approaches. These modeling activities are **closely inter-linked with experimental studies** within the MA department as well as outside MPIE.

To predict the **ductility of materials**, we systematically search for suitable figures of merit. An example is our activities in the case of Mg alloys [5,11] where we connect (i) atomic-scale compositional changes and (ii) an experimentally detected increase in the ductility where yttrium and/or selected lanthanides are used as solutes (see highlight on p. 111 with the MA department - S. Sandlöbes, S. Zaefferer, and D. Raabe). Our goal is not only to understand how Y and lanthanides additions influence the ductility of Mg but also to suggest which other solutes can possibly be used as more accessible and environment-friendly alternatives to them (L.-F. Zhu, Z. Pei, in cooperation with C. Race, A. Dick, G. Leyson and within the AICES program p. 31).

As far as the **strength of materials** is concerned, solid-solution strengthening of Al has been studied and fundamental anti-correlations between the thermodynamics-governed solubility of solutes and their strengthening impact have been quantitatively described (cooperation with D. Ma and D. Raabe). Employing the volumetric mismatch between the matrix and solutes as the decisive parameter, an optimum volumetric mismatch (that can be connected with specific chemical elements from the periodic table) has been predicted for any given annealing temperature (see Fig. 7).

As one of the recently accomplished **methodological developments**, an open-access web-based application calculating integral elastic response of texture-free multi-phase polycrystalline materials has been successfully implemented (H. Titrian and U. Aydin). The new software tool called SC-EMA (**S**elf-consistent **C**alculations of **E**lasticity of **M**ulti-phase **A**ggregates) is based on an easily extendable Python modular library (www.mpie.de/SC-EMA.html). The package uses single-crystalline elastic constants $C_{ij}$ as input parameters and calculates macroscopic elastic moduli (bulk, shear and Young's) and Poisson ratio of both single-phase and multi-phase aggregates employing self-consistent mean-field methods. Crystallites forming the aggregate can be of cubic, tetragonal, hexagonal, orthorhombic, or trigonal sym-

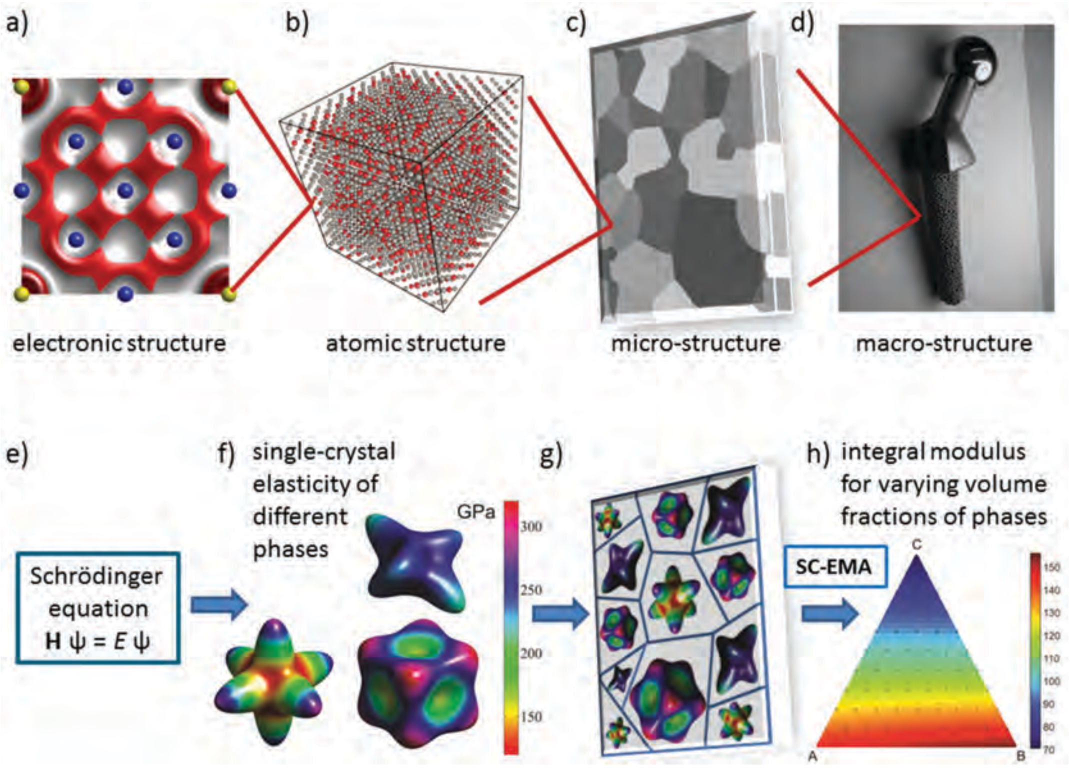


**Fig. 6:***Relation between the multi-scale structure of a material (a)-(d), represented here by a stainless steel hip-replacing medical implant (d), with the corresponding modeling approaches to determine elastic properties (e)-(h). Part (h) shows a triangular plot of the homogenized Young's modulus of a 3-phase aggregate for different volumetric fractions of phases as calculated and visualized by a newly developed software tool SC-EMA (**S**elf-consistent **C**alculations of **E**lasticity of **M**ulti-phase **A**ggregates), (H. Titrian and U. Aydin).*

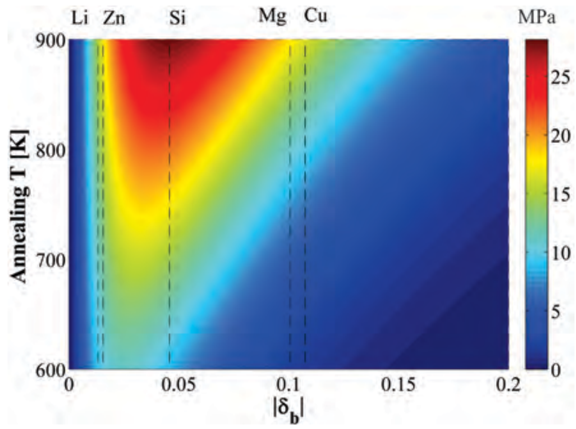
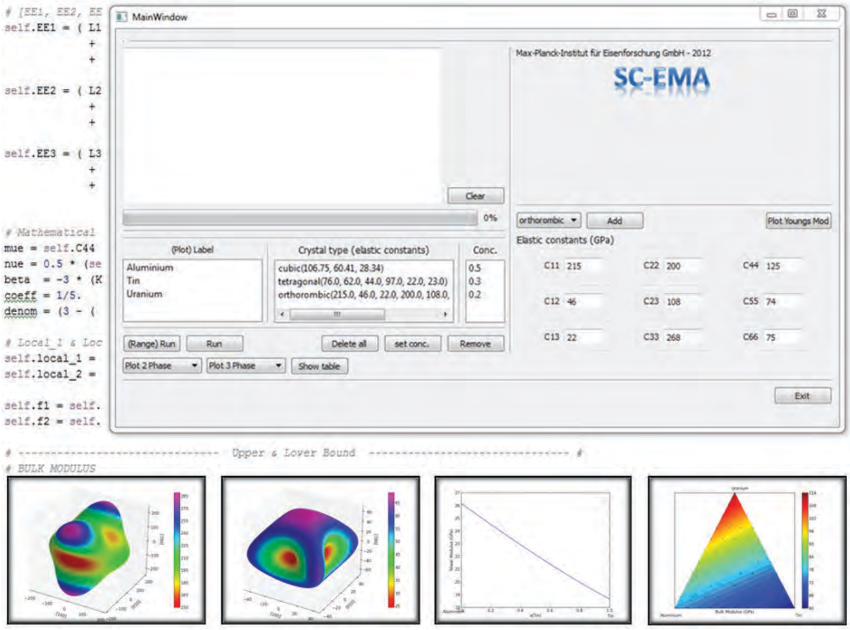


**Fig. 7:** *Color-coded contour plot of the yield stress (in MPa) of polycrystalline Al solid solutions, $\sigma_y$ measured at 78 K, on annealing temperature T and dimensionless volumetric mismatch $|\delta_b|$ = 1/a * (da/dc) as a function of the lattice parameter a and solutes concentration c (in collaboration with MA department - D. Ma and D. Raabe). Also indicated are volumetric mismatch values corresponding to a few industrially used Al-strengtheners.*

metries. In case of multi-phase polycrystalline composites, the shear and bulk moduli are computed as a function of volumetric fractions of phases present in the aggregate (see Fig. 8). The application has built-in criteria that are checking the mechanical stability of phases based on input single-crystalline elastic constants. Elastic moduli are computed together with their bounds as determined by Reuss, Voigt and Hashin-Shtrikman homogenization schemes. From an engineering point of view, the newly developed software probes in a scale-bridging manner fundamental structure-property relations and can be used as a **toolkit for materials-design simulations of alloys with specific macroscopic elasticity**.



```
# [EE1, EE2, EE
self.EE1 = ( L1
             +
             +

self.EE2 = ( L2
             +
             +

self.EE3 = ( L3
             +
             +

# Mathematical
mue = self.C44
nue = 0.5 * (se
beta  = -3 * (K
coeff = 1/5.
denom = (3 - (

# Local_1 & Loc
self.local_1 =
self.local_2 =

self.f1 = self.
self.f2 = self.

# ------------------------------ Upper & Lower Bound ------------------------------ #
# BULK MODULUS
```

MainWindow

Max-Planck-Institut für Eisenforschung GmbH - 2012

SC-EMA

| (Plot) Label | Crystal type (elastic constants) | Conc. |
|---|---|---|
| Aluminium | cubic(106.75, 60.41, 28.34) | 0.5 |
| Tin | tetragonal(76.0, 62.0, 44.0, 97.0, 22.0, 23.0) | 0.3 |
| Uranium | orthorombic(215.0, 46.0, 22.0, 200.0, 108.0, | 0.2 |

orthorombic

Elastic constants (GPa)

C11 215
C22 200
C44 125
C12 46
C23 108
C55 74
C13 22
C33 268
C66 75

**Fig. 8:** *Screen shots of the newly implemented SC-EMA package intended for analyzing single-crystalline elasticity of crystals with arbitrary symmetry and mean-field calculations of integral elastic response of single and multiple-phase aggregates.*

Further research activities focus on e.g. **multi-methodological approaches combining quantum-mechanical and/or atomistic simulations with continuum methods** such as crystal elasticity and crystal plasticity finite element method (CEFEM and CPFEM) together with the MA department, new fast Fourier transforms (FFT) approaches (cooperation with R. Lebensohn, Los Alamos National Laboratory, USA), and phase-field modeling (with H. Emmerich, Bayreuth University), see details e.g. in [12]. As far as various methodological aspects are concerned, different computational methods to the second-order elasticity of cubic crystals were compared and the numerically most robust approach (that also allows for calculating the third-order elastic parameters) was identified [35] (cooperation with D. Holec and P. Mayrhofer from the University of Leoben, Austria).

***Ab initio* calculations** were also applied to a wide range of materials and phenomena, such as (i) changes induced in stoichiometric NiTi allotropes by hydrostatic pressures [36] (together with D. Holec, University of Leoben, and A. Dlouhý, Institute of Physics of Materials (IPM) in Brno, Czech Republic), (ii) the role played by magnetism in martensitic phase transformations (e.g. in Ni, Fe and Co) [4,37] with M. Zelený (Aalto University School of Science, Finland) and M. Šob (IPM and Masaryk University in Brno, Czech Republic), as well as (iii) DFG-funded research focused on two-phase Ti−Fe eutectics [38,39], or Ti−Nb alloys for bio-medical applications [13]. New ways of designing multi-phase materials with extremal strength-to-weight ratios were studied within a biomimetic research aiming at complex hierarchical biocomposites (P. Elstnerová, formerly also with M. Petrov) [14,40] together with H. Fabritius from the MA department, A. Ziegler from the University in Ulm, S. Nikolov from the Bulgarian Academy of Sciences in Sofia, and Z. Střelcová from the Central European Institute of Technology, Brno, Czech Republic. This collaborative DFG-funded project has been successfully defended after the first two-year-long funding period and its extension till May 2013 was approved in early 2011.

The long-term development of the group, that was established in June 2005, can be characterized by systematic building up of knowledge in (i) revealing intrinsic relations between thermodynamic and mechanical properties of materials (jointly with CPS group), (ii) describing the elasticity of materials, earlier only single-phase and ordered ones, subsequently disordered alloys (together with J. von Pezold and A. Dick) [41] as well as multi-phase composites, and (iii) going beyond the elasticity of materials towards their plasticity that is more important for industrial applications. All this accumulated knowledge has been used to (i) explain trends in existing materials when inter-linking theoretical and experimental studies both inside and outside the MPIE, (ii) explore limits of materials design of new alloys, (iii) establish new multi-methodological connections among different modeling approaches, and (iv) ultimately also design new materials, such as new ferritic steels intended for high-temperature applications developed within the BMBF-funded project “Ferrit950” (a patent application involving MPIE as a co-proposer is pending).

### Defect Chemistry and Spectroscopy (C. Freysoldt)

The 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 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. Major challenges in the simulation arise from (i) 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, (ii) linking the microscopic picture to a coarse-grained theory that is able to describe the experimentally relevant time and length-scale (scale bridging), and (iii) developing useful approaches for point defects in amorphous/disordered materials.

The group heads and coordinates the development of our in-house **multi-scale program package SPHInX.** In the past two years the focus has been on parallelization of key algorithms using MPI and openMP as well as on the public release of the source code (version 2.0) [6]. The MPI parallelization was implemented in collaboration with the MPG Computing Center in Garching, and follows an adaptable single-loop parallelization model. The collaboration revealed again the power and efficiency of the SPHInX modular concept, since the implementation was finished within a few weeks(!) by K. Reuter (GRZ Garching), a plasma physicist by training who admitted to have no real understanding of electronic-structure theory. He highly praised the conceptual clarity of the SPHInX code. Further external collaborators on SPHInX development are Sixten Boeck (Gemmantics IT Consulting, Erkrath) and Oliver Marquardt (Paul-Drude-Institut, Berlin). Recent in-house developments cover a mixed Coulomb-Hook formalism for coarse-graining phonon calculations in (defective) ionic systems, calculation of energy loss near-edge spectra (S. Zhang), orbital-based energy decomposition using Quamols (B. Lange), and hybrid functionals. Apart from being an efficient platform for method innovation, the SPHInX code is now routinely used for applied research throughout the department.

A unique module in the SPHInX package is the **plane-wave based implementation of k·p theory** that allows to efficiently calculate electronic states as well as strain in semiconductor nanostructures. The implementation offers full flexibility in terms of underlying model Hamiltonian, material composition, and shape of the nanostructure, which are all defined in easy-to-edit input files [33,34]. The code is now being routinely applied – also outside the institute – to a variety of nano-structured semiconductors such as quantum dots, quantum dot arrangements (‘quantum camomilla flowers’), and even to states trapped by the strain fields of extended defects (O. Marquardt, Paul-Drude-Institut, Berlin).

An important aspect of our fundamental research is to provide physically clear interpretations of the quantitative and qualitative results obtained for specific systems. These insights provide important landmarks in guiding applied research towards promising directions. Based on our recent **development of optimized atomic orbitals (Quamols)** [37], that accurately represent the results of highly accurate plane-wave calculations, we are now able to decompose not only wavefunctions and electronic band structures into their atomic contributions, but also the resulting energies. This **new analysis tool** is applicable to a wide range of unsolved question such as the energy distribution in alloys and amorphous materials, surface energies of polar surfaces or the origin of the energetics of defects. Additionally, it provides a very direct and intuitive approach to draw the border line between the bulk and the region nearby the defect that is already modified from its bulk-like behavior. The new approach is also ideally suited to design coarse-grained empirical models for embedding, where the defect region is re-parameterized according to *ab initio* calculations (B. Lange).

Inspired by the successful calculation of **finite-temperature *ab initio* thermodynamics** for bulk metals, we extended the method to **defects in oxides** within a visiting PhD student program financed by the Chinese Ministry of Education. A major challenge arises from long-range Coulomb interactions that render the direct approach of deriving the dynamical matrix from a series of force calculations impractical. Splitting the interatomic interactions into a long-range Coulomb part and short-range harmonic corrections restores the locality of the phonon model parameters. This locality makes the model amenable to parameterization from DFT and holds not only for ionic bulk materials, but even for charged defects. First results for the oxygen vacancy in MgO show that the presence of a defect modifies the effective charges of nearby atoms in a non-trivial way: as the local symmetry is broken, the apparent charge becomes dependent on the direction in which the atom moves. The vacancy has dramatic consequences for the phonon density of adjacent shells, and hence the vibrational free energy derived from it. The contribution of zero-point vibrations to the free energy can be as large as 0.1 eV − a magnitude that one only would expect for the lightest of all atoms, i.e. hydrogen. The vibrational entropy is even enhanced upon vacancy formation − counter-intuitively, since in total, three degrees of freedoms are lost. These surprises highlight that the common assumptions on the (un) importance of vibrations for formation energies need be revised for defects (J. Wang).

On the **methodological side**, we were able to show in collaboration with Chris Van de Walle (University of California, Santa Barbara) that major discrepancies in calculated defect energies with traditional LDA/GGA functionals and more recent hybrid functional calculations can be largely resolved by the consequent application of charge corrections and realignment of the calculated band structure to deep charge transition levels [42]. Applying these techniques allowed us to understand the doping limiting mechanisms in optoelectronic materials and to revise the conventional doping picture by a new one that is consistent with recent experimental findings [43] (B. Lange). These activities are part of our collaboration with OSRAM.

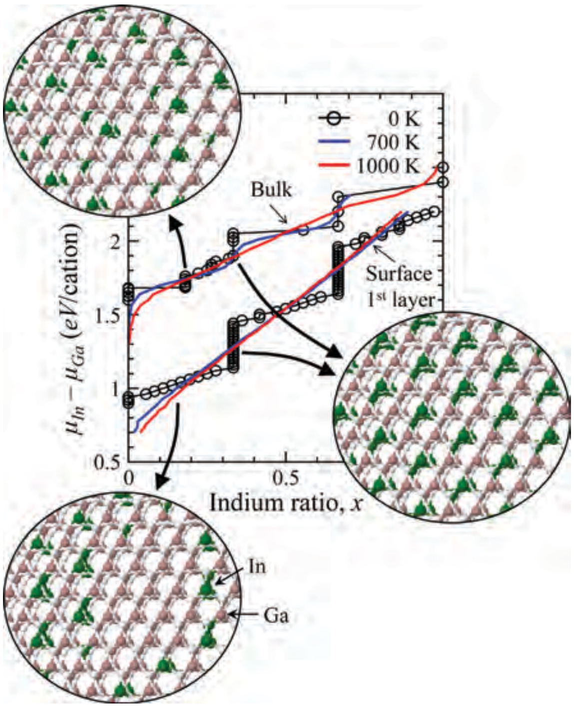


**Fig. 9:** *Ordering phenomena and thermodynamics for wurtzite* $In_xGa_{1-x}N$ *alloys, epitaxially constrained to GaN. The graph shows the chemical potential for a bulk material and a 3-layer thin film covered by an In adlayer. Insets highlight the corresponding ordered structure at 0 K. Thin films not only show a much higher tendency to incorporate indium, they can decompose laterally into ordered phases. This is enabled by vertical relaxation near the surface that is elastically suppressed in thicker films.*

The state of the art of defect calculations has now reached the point where it is high time to push forward their application to fields that previously seemed inaccessible due to the required accuracy of prediction. We have therefore organized in late 2011 **a workshop to bring together leading theoreticians from solid state theory and electrochemistry**. In a thriving atmosphere of inspired discussions, the participants shared their knowledge on a number of common key questions such as the inclusion of long-range electric fields due to charged defects, that are looked at very differently from each field's historical perspective.

The dangling-bond defect in hydrogenated amorphous silicon, that we study in the 5-year EPR Solar network project funded by the German ministry of research, is a prime example of a **defect in an amorphous/disordered system** (see p. 151). Our detailed analysis of the EPR parameters of this defect in comparison to dangling-bond-like defects in crystalline silicon has revealed how the specific characteristics are intimately linked to those of the amorphous matrix [44] and helped to interpret the experimental EPR spectra in terms of local structures. In contrast to previous work based on a rather idealized, textbook picture of a dangling bond, we show that the observed red-shift of hyperfine satellites results from an electronic delocalization, intrinsic to amorphous silicon, rather than a geometry-induced rehybridisation [45] (G. Pfanner).

To better understand the properties and growth of **ternary nitride alloys for optoelectronic device applications**, 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. The underlying empirical potentials were parameterized from DFT calculations and capture the relevant chemical and elastic interactions. Our results show a strong tendency for next-nearest neighbor ordering, culminating in ordered alloys at 33% and 66% In concentration, see Fig. 9. Alloys of intermediate concentrations can be understood in terms of patches of these ordered phases. It is currently investigated if this notion can be used to construct reliable continuum models with nanoscale composition fluctuations that can be parameterized from the ordered phases only (S. Lee).

### Adaptive Structural Materials (B. Grabowski)

The Adaptive Structural Materials (ASM) group established in April 2012 has a unique construction within MPIE: It is a hybrid theoretical-experimental group where an equal number of scientists from the CM and MA department work jointly together (see also *New Research Groups*, p. 13). The special task of the ASM group is to foster and further optimize the already intensive interdepartmental collaborations to a yet greater extent. To address the needs of such a mixed group, the theoretical unit of ASM has to cover a **wide scope of computational techniques and methodological tools**.

The backbone of ASM's applied research is closely related to the ERC SMARTMET project (see *Large Scaled Projects*, p. 25). The main aim is to boost next-generation **mechanical properties beyond present limits**. The key to this is a well-controlled application of intrinsic phase instabilities. Thus, an accurate and efficient determination of free energies, which determine stability regimes, is of central importance. The group has therefore strong ties to the group "Computational Phase Studies" (CPS, p. 38) and method development related to this topic is done in well-arranged collaborations. In these collaborations the ASM group has its main focus on the description of **instabilities and anharmonic contributions**. An example is the co-supervision of the project of D. Korbmacher (ASM) by A. Glensk (CPS) where previously developed *ab initio* methods [3] are extended to enable a highly accurate description of **temperature driven phase transitions** in Ti-alloys.

Another example is the co-supervision of the project of L. Xu (ASM) by F. Körmann (CPS) where the separately developed methods for describing anharmonicity and spin excitations are coupled. This will allow a much more **precise description of steels at high temperatures**. A backward flow of knowledge (ASM to CPS) is likewise established, for instance, by the input of ASM's expertise (B. Grabowski) into an accurate description of **point defects up to melting temperature** including all relevant finite temperature excitations (see p. 147) [22].

The **Gum Metal project** (see p. 113) is a first concrete application of the ideas behind SMARTMET. Specifically, Ti–Nb based alloys are considered which acquire special mechanical properties due to an extreme softness of their elastic constants. The work on Gum Metal is done in direct collaboration with the experimental part of the ASM group (C. Tasan, MA department). First achievements are related to revealing new plasticity mechanisms and to establishing the importance of oxygen. Future theoretical steps will be directed towards calculation of instability phase diagrams which are crucial in determining the Gum Metal effect (L. Huang).

Another attempt to overcome present mechanical limits is pursued within the **nano-pearlite project** (see p. 107). Nano-pearlite reaches the highest strengths ever achieved for a structural alloy, making it highly attractive to understand the underlying mechanisms. The project requires an intensive collaboration with experimentalists (Y.J. Li, MA department) and the development and application of a wide range of simulation tools. Important theoretical results include the *ab initio* based determination of the thermodynamic driving force for carbon redistribution [46]. Present investigations concentrate on the influence of dislocations where drag effects are simulated using the nudged elastic band method and molecular dynamics employing empirical potentials (A. Nematollahi).

A third pillar of the ASM group is the **hydrogen enhanced local plasticity (HELP) project** aiming at understanding and eventually overcoming hydrogen embrittlement. Tackling the challenges related to H embrittlement is a tremendous effort requiring expertise from various fields. The project is therefore pursued in close collaboration with the "Mesoscale Simulations" and "Computational Phase Studies" group (both CM department). Additionally, a close link to the group R. Kirchheim from the University of Göttingen exists, which recently led to a joint DFG proposal application on this topic. The focus of the ASM group within the HELP project lies on extending the previously developed methodology [47] to iron based systems and to provide a validation of the empirical potential simulations with *ab initio* methods. To this end, the ASM group was recently joined by an expert in such calculations (G. Leyson).

To provide the necessary technical basis for the above projects, strong activities in method development are undertaken. The guiding principle can be summarized as **highest accuracy with minimum computational time**. The accuracy aspect is tackled at various length and time scales. At the smallest scale, the typically applied *ab initio* methods in form of density functional theory, which are limited by the approximation to describe exchange-correlation, are extended towards an even more fundamental approach, the **Quantum Monte Carlo approach**. In collaboration with M. Morales-Silva from the Lawrence Livermore National Lab the possibility of establishing a Gold Standard for *ab initio* simulations of metallic systems with Quantum Monte Carlo is investigated.

On the density-functional-theory level, the ASM group strives to further increase the accuracy/efficiency ratio in calculations of the computationally demanding **anharmonic contributions** important for phase stability (D. Korbmacher, L. Huang). On the empirical potential level, efforts are undertaken to increase the accuracy of presently available **embedded atom potentials** (M. Grabowski).

In its development, the ASM group significantly profited from projects (*e.g.*, nano-pearlite and HELP) that were inherited from a former group of the CM department (Microstructure, J. von Pezold). A special highlight that grew up in the former group and is now successfully hosted in the ASM group provides new and exciting insights about grain boundary motion (C. Race, see p. 121). These projects quickly got ASM under way. Two new projects will start within the next few months. O. Vekilova will contribute her expertise in calculating ***ab initio* elastic constants at finite temperatures** to ASM's efforts related to the SMARTMET project. L. Huber will join from a group specialized in multiscale modeling of microstructure evolution (M. Militzer, University of British Columbia). He will work within a DAAD research fellowship on the **influence of solutes on grain boundaries in iron**.

### Mesoscale Simulations (R. Spatschek)

The research in the group is devoted to the understanding of **phenomena appearing on dimensions between the atomic and continuum scales**. As a generic feature the microstructure of a material intrinsically links these scales, thus naturally connecting to the other groups within the department and institute. Various computational and analytical techniques, which are particularly tailored to the different applications, are used in the group. The further development and improvement of models and simulation techniques is also an important activity. In the following, recent key activities in the group are briefly discussed.

A fascinating research area, which has attracted intense interest during the past years is related to **grain boundary premelting**. Here, depending on the type of the grain boundary and the local misorientation, a melt film can form along the grain boundary already below the bulk melting point. It therefore has tremendous influence on the stability of materials at elevated temperatures and affects dendrite coalescence and microstructure evolution. Understanding this phenomenon demands to link mesoscale thermodynamic concepts to atomic scale elastic distortions due to the presence of misfit. We used phase field crystal and Ginzburg-Landau techniques, which are related to classical density functional theory, to predict this material failure mechanism. We shed light on the role of the underlying short range structural disjoining forces, also in conjunction with thermal noise. In particular, we were able to extract the asymptotic behavior of the disjoining potential, leading to a fully analytical prediction of the gamma surfaces close to the melting point. Presently, we link these findings to the kinetics of **liquid metal embrittlement**, which is a major problem e.g. for welding of zinc coated steels. Here, we model the melt invasion along a grain boundary taking into account the aforementioned structural forces, in combination with aspects of crack propagation [48-51] (C. Hüter, F. Twiste).

Further activities are related to the field of **heterogeneous nucleation and microstructure evolution**, embedded into the DFG priority program 1296. Our aim is to understand the role of elastic effects both on the initial regime of nucleation as well as the long time evolution of microstructures. Recent activities are related to the growth of **nanowires**. Here we studied in particular the competing elastic and interfacial effects, which limit the aspect ratio of the forming nanowire. Also, we investigated so called pine tree nanowires, which are grown around a screw dislocation in their center and generating a twist of the wire around this axis. The arising internal elastic stresses destabilize the wire and favor the Rayleigh-Plateau decomposition into droplets [52,53] (G. Boussinot, R. Schulz).

We studied **solidification** of monotectic and syntectic alloys, which are relevant for lead-free soldering. The common feature of both systems is the appearance of phase separation in the melt phase, allowing for phase coexistence of two liquid and one solid phase. The steady state growth has been analyzed theoretically using Green's function methods and phase field techniques (see Fig. 10). The outcome of these studies is the prediction of the growth velocity and length scales of the emerging microstructures, depending on the undercooling and alloy composition [54] (G. Boussinot, C. Hüter).

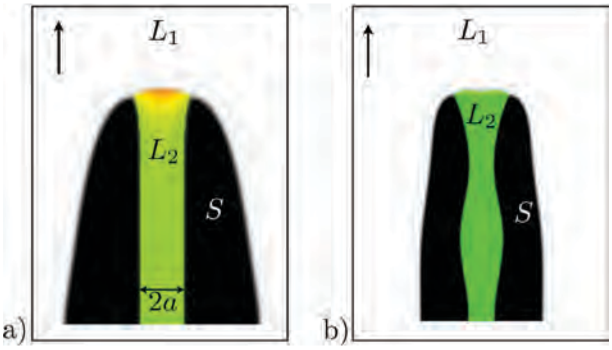


**Fig. 10**: *Solidification of a monotectic alloy. Two-phase finger with the solid (black) surrounding the liquid $L_2$ (green/grey) in a) steady state, b) oscillatory regime. The arrow indicates the growth direction.*

The Ginzburg-Landau methods, which link atomistic modeling to large scale mesoscale phase field simulations, have also been used to study grain boundaries in bcc $\delta$-iron near the melting point. In agreement with phase field crystal and molecular dynamics simulations we find a transition between a state of paired edge dislocations and a splitting into individual dislocations with a mixed edge end screw character at lower temperatures (see Fig. 11). This **dislocation pairing transition** is an important benchmark for the rather recently developed Ginzburg-Landau model in our group. The underlying codes, which have been developed in our group, are run efficiently on GPUs, with an acceleration up to a factor 250 in comparison to a single core CPU code [55] (C. Hüter).

Another important reason for material failure in high-strength steels is **hydrogen embrittlement**. Our focus here is on hydride forming materials, which nucleate a hydrogen-saturated region in particular near defects like edge dislocations and therefore favor a ductile-to-brittle transition. As a prototype we simulated the Ni−H system using Monte-Carlo simulations and molecular statics. The full quantitative linking to a macroscopic and thermodynamic description, taking into account nonlinear elastic effects opens the path for a true and quantitative scale bridging modeling of material failure. The elaborated free energy model can directly be used e.g. in phase field models and is presently used to predict the stress induced hydride formation at crack tips. This project is part of the DFG Collaborative Research Center 761 "Steel *ab initio*" [9] (D. Korbmacher, J. v. Pezold, C. Hüter).

A more methodological development is pursued in the coupling of **phase field models with plasticity**. In many transformations in steels stresses reach rather high values such that plastic deformations are involved. We have worked out a general framework that couples these two aspects, focusing on the issue of internal variables describing the plastic state. It turns out that the evolution equations for front propagation do not follow uniquely from variational principles [56].

**Phase change materials** are exciting candidates for fast and nonvolatile data storage. The basic concept is a phase transformation between an amorphous and a crystalline state, triggered by the heat generated by an electrical current. The different conductivities between the phases allow to distinguish between the phases and thus to store information in the memory cell. In this project we focus on the kinetics of the switching process, and we developed a phase field model to simulate the Joule heating induced phase front propagation. In order to overcome the high computational cost of these simulations, a GPGPU implementation has been implemented, leading to a code acceleration by two orders of magnitude in comparison to a conventional CPU code. This activity is linked to the DFG Collaborative Research Center 917 "Nanoswitches" [57,58] (G. Boussinot, A. Monas).

## Other Activities

### Corrosion, Surface and Interface Related Activities (M. Todorova)

Processes occurring at surfaces or interfaces of materials can influence their properties in a multitude of different ways. Examples are embrittlement, corrosion or catalytic reactions, which might be desired or not, depending on a targeted functionality. Various activities have been initiated and supervised by M. Todorova:

In the manufacturing of high quality steel products, processing steps and costs can be reduced by hot-forming of already coated steel plates. Such a process has been observed to lead to degradation of the quality of work pieces, caused by **liquid metal embrittlement** of bulk steel coming into contact with liquid zinc. The mechanisms underlying this process were investigated in the diploma work of K.-D. Bauer in a collaborative effort involving the Zentrum für Oberflächen und Nanoanalytik, Johannes Kepler University Linz (K. Hingerl). Combining DFT with a modified Griffith model we were able to explain the liquid metal embrittlement in the hot-forming process of galvanised steel: Zinc is found to wet grain boundaries and to promote fracture along them, by significantly reducing the costs for crack propagation – even a single monolayer of zinc decreases crack propagation cost in a $\Sigma3$ grain boundary by 22% and in a (more realistic and suggested by experiment) $\Sigma5$ grain boundary by 43% (K.-D. Bauer).

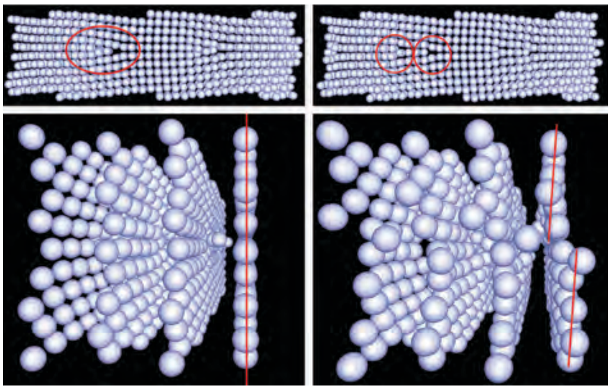


**Fig. 11**: *Symmetric tilt in bcc δ-iron. At high homologous temperatures of more than about 85% of the melting temperature the dislocations have a pure edge character (left panel). For lower temperatures they split into partials with additional screw character, leading to out-of-plane deformations. Top row: View onto the grain boundary. Bottom row: View along the grain boundary.*

Stoichiometric **iron aluminides** are candidate materials for high temperature applications, but their applicability is impeded by a poor room temperature ductility caused by **environment-induced embrittlement**. It has been suggested in the literature that both addition of suitable alloying elements, as well as the presence of passive surface films may reduce the problems caused by hydrogen. Aiming to understand the effects either of these processes may have, we focus on $Fe_3Al$. On one hand we investigate the preferential surface terminations of the clean surfaces and their interactions with oxidising species, which will allow us to identify changes in the surface behaviour upon addition of alloying elements. On the other hand, we look into both the coupling to the substrate and the stabilisation subject to the environmental conditions (employing surface phase diagrams) of passivating $Al_2O_3$ (A. Izanlou).

Magnesium is one of the lightest metals with potential applications ranging from automotive, to aerospace to medical applications. Understanding the **corrosion behaviour of Mg and its alloys**, when in contact with an oxidising environment is important for any of these (applications) and serves as important model system for other materials. Performing DFT calculations for Mg in contact with different oxidising species (N, O, F and Cl) allowed us to address the propensity of Mg to oxidise and identify similarities and differences in its behaviour towards the different oxidising agents (S.-T. Cheng).

**Corrosion in sour gas media** is a particular problem for low-alloyed steels. Iron-sulphide layers which form under the influence of the sour gas environment have been observed to sometimes have a beneficial effect by providing a diffusion barrier for further penetration of harmful species. Morphology and stability of the capping layer are hereby of central importance. We aim to gain a deeper insight into the interactions, which lead to the formation of **Fe−S layers at the surface**, address their composition and structure, and understand the mechanisms and conditions which influence their passivating function. The gained insight is expected to aid systematic improvement of the corrosion properties of low-alloyed steels in sour gas media (M. Ilhan, to start on 1 Jan. 2013).

### Epitaxy and Surface Characterization (L. Lymperakis)

Group III-Nitrides and their ternary alloys are materials of choice for high temperature and high power microelectronic devices which are of special interest for the automobile industry as well as for solid state lighting (SSL) and chemical and biological sensor applications. L. Lymperakis is involved in two EU funded projects: (i) The Industry-Academia Marie-Curie project SINOPLE and (ii) the Nanosciences, Nanotechnologies, Materials and new Production Technologies project ALIGHT. Topics that are addressed in this area are:

The growth of high In content as needed to access the green region of the spectrum and high quality InGaN films is challenging: The size difference between In and Ga as well as the difference in In−N and Ga−N bond strengths has been suggested to result in In surface segregation, limited In incorporation as well as **spinodal decomposition and phase separation**. To overcome these obstacles low growth temperatures are commonly used that however result in rough surface morphologies and impaired crystal quality. Using *ab initio* techniques, we have **computed surface growth diagrams** showing the most stable structures as function of the growth conditions. These calculations naturally include **surface segregation** effects and allow to identify optimum growth conditions (A. Duff).

High resolution transmission electron microscopy (HRTEM) imaging combined with a subsequent strain analysis allows **to map the HRTEM measured lattice parameter into a local chemical composition**. Conventional approaches, however, assume for the underlying analysis a homogeneous and linear elastic medium. Since in actual HRTEM very small volumes are probed, atomic scale effects may become important. We have therefore combined large scale modified embedded atom method (MEAM) calculations with HRTEM experiments and image simulations on ternary $In_xGa_{1-x}N$ Quantum Wells (QW) embedded in a GaN matrix. Our approach revealed that these alloys are structurally inhomogeneous on the atomic scale and exhibit strong interactions between adjacent cells. Both effects may result in misinterpretation of the HRTEM images such as erroneous chemical clustering (A. Duff, in cooperation with M. Albrecht, Leibniz Institute for Crystal Growth, Berlin).

**Scanning tunneling microscopy (STM)** is commonly believed to offer an **exceptional sensitivity to surface states** combined with unprecedented atomic resolution and constitutes one of the most appropriate methods to probe the surface atomic and electronic structure. Addressing an on-going controversial debate regarding the electronic structure of non-polar GaN surfaces we could demonstrate that under certain conditions surface states may be fully shadowed by bulk states and invisible in normal STM operation modes. Based on this insight and using the *ab initio* computed bandstructure we designed a new STM operation mode that our experimental partners successfully used to probe and identify hidden surface states (in cooperation with Ph. Ebert, Peter Grünberg Institut, FZ Jülich GmbH).

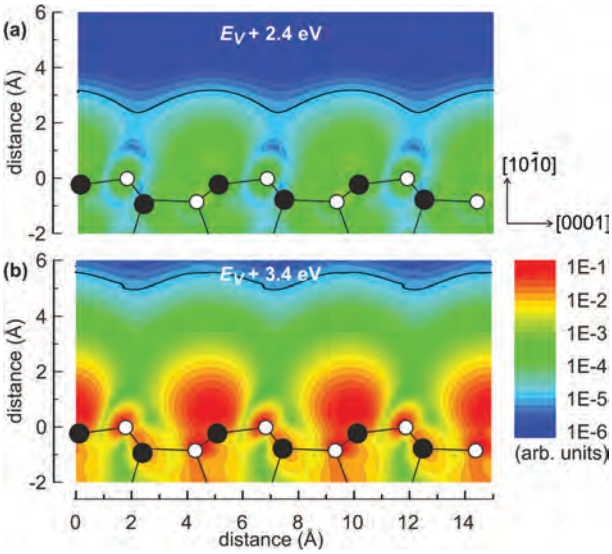


**Fig. 12:** *Spatially resolved density of states as seen by an STM at two different tunnel voltages for the example of a GaN* $(1\bar{1}00)$ *surface. The fast decay of the surface states into vacuum is clearly seen and results in low (bulk like) corrugation at typical surface-tip distances (black line).*

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## Research Projects in Progress

**Computational Phase Studies**

*Dutta, Hickel, Neugebauer (in collaboration with K.R.A. Ziebeck*, K.U. Neumann*, P. Entel** (*Loughborough University, UK, **Univ. Duisburg-Essen)): Ab initio* investigation of temperature dependent effects in shape memory Heusler alloys

*Dutta, Hickel (in collaboration with A. Hütten*, I. Opahle**, G. Madsen**, R. Drautz**, A. Waske*** (*Universität Bielefeld, **Ruhr-Universität Bochum, ***IFW Dresden)): Ab initio* study on the coupling of lattice and magnetic degrees of freedom and the role of interfaces in magneto-caloric materials

*Aydin, Hickel, Neugebauer (in collaboration with R. Drautz, ICAMS Bochum):* Chemical trends for the solubility and diffusion of hydrogen in metals with high-throughput calculations

*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

*Körmann, Hickel, Nematollahi, Grabowski, Neugebauer (in collaboration with S.V. Okatov*, Yu.N. Gornostyrev*, A. Leineweber** (*Ekaterinburg, Russia, **MPI Stuttgart)):* Formation of $Fe_3C$ precipitates in ferritic steels

*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

*Körmann, Hickel, Neugebauer (in collaboration with M. Palumbo*, S. Fries*, B. Hallstedt** (*ICAMS, Bochum, **RWTH Aachen)): Ab initio* simulation of magnetic contributions to the thermodynamics of metals,

*Nazarov, Hickel, Neugebauer (in collaboration with L. Duprez*, R.G. Thiessen**, K. Mraczek***, H. Hänninen****, Y. Yagodzinskyy**** (*OCAS, Belgium, **TKS, Duisburg, ***VoestAlpine, Austria, ****Aalto Uni, Finland)):* Hydrogen sensitivity of different advanced high strength microstructures

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

*Dey, Nazarov, Hickel (in collaboration with D. Mirkovic, T. Evertz, F. Klose, Salzgitter Mannesmann Forschung GmbH):* Investigation of hydrogen and carbides in HSD steels

*Zhang, Hickel, Neugebauer (in collaboration with J. Rogal and R. Drautz, Ruhr-Universität Bochum):* The role of interfaces for the martensite formation in steels

*Körmann, Grabowski, Hickel (in collaboration with S. Fries, Ruhr-Universität Bochum):* Sapiens – Thermodynamic modeling of unary metals

*Hickel, Friák, Neugebauer (in collaboration with Y. Gornostyrev, CJSC Inistitute of Quantum Materials Science, Ekatarinburg): Ab initio* prediction of thermodynamics and kinetics of clustering in maraging steels

*Hickel, Körmann (in collaboration with E. Povoden-Karadeniz, Institute of Materials Science and Technology, Vienna):* Thermodynamic modeling of TCP phases

*Körmann, Hickel, Neugebauer (in collaboration with Z.-K. Liu, Pennsylvania State University):* Modeling of paramagnetic properties of metals

### *Ab Initio* Thermodynamics

*Friák, Neugebauer (in collaboration with G. Brückner*, H.H. Angermann**, B. Sahebkar***, B. Kuhn****, H. Hattendorf*****, S. Weber****** (*ThyssenKrupp Nirosta GmbH, **Behr GmbH & Co. KG, ***Benteler Automobiltechnik GmbH, ****Forschungszentrum Jülich, *****ThyssenKrupp VDM GmbH, ******Ruhr-Universität Bochum)):* Development of ferritic steels for high-temperature applications („Ferrit950")

*Friák, Neugebauer (in collaboration with J. Eckert*, H. Emmerich** (*Leibnitz-Institut für Festkörper- und Werkstoffforschung Dresden, **Universität Bayreuth)):* Scale bridging studies of the elastic contributions to nucleation and initial microstructure formation in the eutectic system Ti–Fe

*Friák, Neugebauer (in collaboration with A. Ziegler (Universität Ulm) and S. Hild (Johannes Kepler Universität Linz))*: *Ab initio* and atomistic calculation of thermodynamic and mechanical properties of biomaterials

*Friák (in collaboration with M. Šob, Brno): Ab initio* calculations of phase transformations in iron

*Friák (in collaboration with A. Dlouhý*, D. Holec** (*Academy of Sciences of the Czech Republic, **Universität Leoben)): Ab initio* calculations of phase transformations in NiTi

*Friák (in collaboration with M. Zelený, Uppsala University): Ab initio* studies of martensitic phase transformations

*Friák (in collaboration with P.H. Mayrhofer, D. Holec, Universität Leoben): Ab initio* study of hard nitrides

*Friák (in collaboration with M. Šob, Academy of Sciences of the Czech Republic): Ab initio* investigation of Ni-N compounds

### Defect Chemistry and Spectroscopy

*Freysoldt, Pfanner, Neugebauer (in collaboration with F. Finger*, K. Lips**, A. Schnegg**, R. Bittl***, M. Brandt**** (*Research Center Jülich, **Helmholtz-Zentrum Berlin für Materialien und Energie, ***FU Berlin, ****TU München))*: EPR-Solar – Ultra-high resolution EPR spectroscopy on thin film silicon for solar cell research

*Freysoldt, Neugebauer:* Accurate calculation of the electronic structure at grain boundaries via density functional theory and quasi particle corrections

*Freysoldt (in collaboration with S. Boeck*, K. Reuter** (*Gemmantics IT Consulting, Erkrath, **GRZ Garching)):* SPHInX parallelization

*Cui, Freysoldt, Neugebauer (in collaboration with OSRAM Opto Semiconductors GmbH):* Non-radiative recombination at point defects in III-nitrides

*Lee, Freysoldt, Neugebauer*: Ordering effects in epitaxial InGaN alloys

*Lange, Freysoldt, Neugebauer*: Energy decomposition based on Quamols

*Lymperakis, Freysoldt (in collaboration with National University of Ireland, Universität Ulm, University of Cambridge, and Osram Opto Semiconductors GmbH):* ALIGHT: AlGaInN materials on semi-polar templates for yellow emission in solid state lighting applications.

*Lymperakis (in collaboration with Forschungsverbund Berlin e.V. and Topgan Ltd., Warschau):* SINOPLE: Surface engineered InGaN heterostructures on N-polar and non-polar GaN-substrates for green light emitters

### Adaptive Structural Materials

*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 M. Morales-Silva, Lawrence Livermore National Lab, USA)*: Towards a golden standard for first principles calculations in metallic systems

*Grabowski, Glensk, Hickel, Neugebauer: Ab initio* simulations of point defects up to melting: Reconciling theory and experiment

*Grabowski, M., Grabowski, B., Neugebauer*: Improving accuracy of present day's empirical potentials

*Huang, Grabowski, Neugebauer (in collaboration with C. Tasan, D. Ma, S. Sandlöbes, H. Springer, D. Raabe, MA department)*: Theoretical-experimental investigation of Gum metal plasticity

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

*Lei, Grabowski, Körmann, Neugebauer*: Integrated coupling of anharmonic and magnetic excitations

*Leyson, Grabowski, Hickel, Neugebauer (in collaboration with R. Kirchheim, University Göttingen)*: Investigations and calculations of the interaction of hydrogen with dislocations in iron and nickel

*Nematollahi, Grabowski, Neugebauer (in collaboration with Y. Li, MA department)*: Atomic scale analysis of the origin of pearlite's strength

*Race, Neugebauer*: Understanding grain boundary migration

**Mesoscale Simulations**

*Chakrabarty, v. Pezold, Hickel, Spatschek, Neugebauer: Ab initio* based description of hydrogen embrittlement

*Spatschek (in collaboration with H. Müller-Krumbhaar, Research Center Jülich)*: Elastic effects on heterogeneous nucleation and microstructure evolution

*Spatschek (in collaboration with A. Karma, Northeastern University):* Grain boundary premelting

*Spatschek (in collaboration with H. Löwen, Heinrich-Heine-Universität Düsseldorf):* Liquid metal embrittlement and wetting of grain boundaries

*Spatschek (in collaboration with I. Steinbach, Ruhr-Universität Bochum):* Hydrogen at crack tips

*Spatschek (in collaboration with S. Brinckmann, Ruhr-Universität Bochum):* Dual scale modeling of hydrogen embrittlement

*Spatschek (in collaboration with I. Steinbach, Ruhr-Universität Bochum):* Pine tree nanowires

*Spatschek (in collaboration with B. Eidel, Universität Essen):* Phase field modeling with plastic effects

*Spatschek (in collaboration with E. Brener* and M. Apel** (*Research Center Jülich, **ACCESS Aachen)):* Modeling of phase change materials for nonvolatile data storage

*Spatschek (in collaboration with E. Brener, Research Center Jülich):* Pattern formation during solidification and melting

**Corrosion**

*Cheng, Todorova, Friák, Neugebauer (in collaboration with M. Rohwerder, GO department): Ab-initio* investigation of the corrosion behaviour of magnesium and its alloys

*Izanlou, Todorova, Friák, Neugebauer (in collaboration with M. Palm, SN department):* Theory-guided materials design of Fe−Al alloys resistant to environment induced brittleness

*Nykaenen, Todorova (in collaboration with R. Schlögl, MPI Mühlheim):* Platinum surfaces in contact with water

*Todorova (in collaboration with M. Tröger, Salzgitter Mannesmann Forschung GmbH):* Characterization of iron-sulphide layers

*Todorova (in collaboration with K.-D. Bauer and K. Hingerl, Zentrum für Oberflächen und Nanoanalytik, Johannes Kepler University Linz):* Modeling liquid metal embrittlement

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

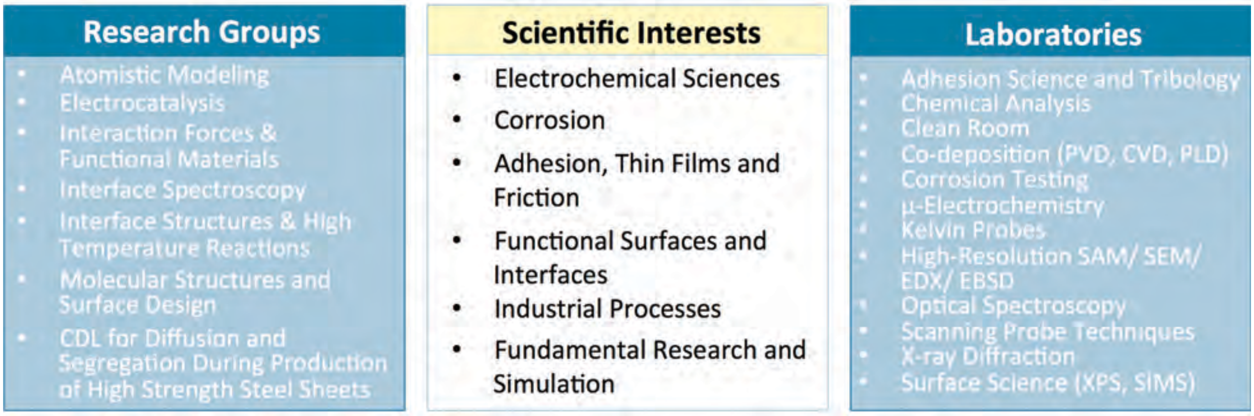
# Department of Interface Chemistry and Surface Engineering

*M. Stratmann*

## Introduction and Retrospective

The Department of Interface Chemistry and Surface Engineering (GO department) is conducting fundamental research in the electrochemical sciences, with a strong **focus on corrosion and adhesion science as well as electrochemical energy conversion.** 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, coatings, nano-porous metallic glasses among others. The department hosts six research groups and the Christian-Doppler-Laboratory (CDL) for Diffusion and Segregation during Production of High Strength Steel Sheet (Dr. M. Rohwerder), which was established in 2008. The different groups focus on high-throughput methods and development of combinatorial methods in adhesion science and electrochemistry, as well as characterization of electrified interfaces by complementary methods such as vibrational spectroscopy, *in-situ* diffraction studies and scanning probe techniques, including Scanning Kelvin Probe (SKP), Atomic Force Microscopy (AFM) or Scanning Tunneling Microscopy (STM). We combine electrochemistry with a surface and interface science approach, and in most projects we complement both, atomically well-defined experimental studies and experiments with real systems by atomistic *ab initio* and larger-scale (continuum theory) 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 last 6 years the group structure of the department was subject to a number of advancements and adjustments: In 2007, Prof. G. Grundmeier (head of the former Thin Films Group) was appointed full professor and chair of the Department for Technical and Macromolecular Chemistry at the University of Paderborn (UPB, Germany). Also in 2007, Dr. M. Spiegel (head of the former high-temperature corrosion group) changed to the R&D department of Salzgitter-Mannesmann. As a consequence, two new groups, the Interface Spectroscopy (Dr. A. Erbe), and the Interface Structures and High Temperature Reactions (Dr. F.U. Renner) groups were established in 2007. In 2009, Prof. A.W. Hassel (head of the former Electrochemistry group) was appointed full professor and chair of the Institute for Chemical Technology of Inorganic Materials at the University of Linz (Austria). Accordingly, a new group in the field of Electrocatalysis (Dr. K.J.J. Mayrhofer) could be established. In 2010 the CDL-Laboratory for Polymer/



**Research Groups**

- Atomistic Modeling
- Electrocatalysis
- Interaction Forces & Functional Materials
- Interface Spectroscopy
- Interface Structures & High Temperature Reactions
- Molecular Structures and Surface Design
- CDL for Diffusion and Segregation During Production of High Strength Steel Sheets

**Scientific Interests**

- Electrochemical Sciences
- Corrosion
- Adhesion, Thin Films and Friction
- Functional Surfaces and Interfaces
- Industrial Processes
- Fundamental Research and Simulation

**Laboratories**

- Adhesion Science and Tribology
- Chemical Analysis
- Clean Room
- Co-deposition (PVD, CVD, PLD)
- Corrosion Testing
- µ-Electrochemistry
- Kelvin Probes
- High-Resolution SAM/ SEM/ EDX/ EBSD
- Optical Spectroscopy
- Scanning Probe Techniques
- X-ray Diffraction
- Surface Science (XPS, SIMS)

**Fig.1:** *Research groups, scientific interests and laboratories at the Department of Interface Chemistry and Surface Engineering.*

Metal Interfaces (managed by Prof. G. Grundmeier, UPB) was concluded after 7 successful years.

In the last two years the department had **two further changes of the senior academic staff**. Dr. A.A. Auer (atomistic modelling group) left the institute in February 2012, to establish a modelling group at the Max-Planck-Institute for Energy Conversion in Mülheim. His newly established team collaborates closely with our department in many research projects, such as the correlation of experiment and simulation of adhesion and stability of Pt-nanoparticles on carbon supports and the oxygen reduction mechanism (see p. 129). With the **newly established group in the field of "Interaction Forces and Functional Materials"** (Dr. M. Valtiner) novel experimental setups and laboratories (Surface Force Apparatus and Interaction Forces Laboratory, see p. 16) and competences in particular in the fields of adhesion, friction and bio-functionalization at electrified materials interfaces complement the existing portfolio of the department. As a winner of a BMBF grant (Dr. K.J.J. Mayrhofer), the newly established laboratory for "Differential electrochemical mass spectrometry and gas chromatography" is focused on electrochemical energy conversion and electrochemical reduction of $CO_2$ (see p. 18).

Over the last six years our **efforts in fundamental and complementary industrial research have established a dynamic department with a unique research portfolio and expertise** (see Fig. 1). The department is also actively participating in various collaborative research efforts with internal and external partners. Several scientists of the department are participating in the DFG Cluster of Excellence "Ruhr Explores Solvation" (Resolv), which is centred at Ruhr University Bochum's (RUB) Faculty of Chemistry and Biochemistry. Resolv was awarded in the latest round of the excellence initiative, and commences operation on 1 November 2012. Our contributions to solvation science in Resolv will focus on the role of solvents in electrochemical reactions, and solvation of interfaces (see p. 27). Further, the department is part of a recently awarded EU 7th framework programme Marie Curie Initial Training Network (ITN) under the name of "Somatai - Soft Matter at Aqueous Interfaces". Somatai starts to become reality on 1 October. The Center for Electrochemical Sciences (CES) was founded in collaboration with the RUB in 2009. CES is recognized as a Center of Excellence with the task to ensure international competitive research in all aspects of modern electrochemistry, covering both experimental and theoretical electrochemistry (for details see p. 22).

With its versatile experimental and theoretical expertise (also Fig. 1) the GO department is in the **unique position to assist and promote diverse industrial research areas by the understanding of their 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 GO 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.

The fundamental studies complement the second central focus of our department; the study of electrochemical processes that are of ultimate practical importance in industrial applications. Several research projects focus around phosphating and oxide thin-film growth and properties on engineering metals. 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. The effect of hydrogen in steel, a collaborative interest of the institute, has been investigated by complementary experimental and theoretical methods, and in particular the Scanning Kelvin Probe was further extended to uniquely and directly detect hydrogen in steel with high spatial resolution. The newly developed **Scanning Flow Cell (SFC) coupled to the inductively coupled plasma mass spectrometer (ICP-MS)** allows high-throughput screening of electro-catalysts or corrosion reactions combined with a simultaneous quantification of reaction products.

## 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 overpotential that limits the energy efficiency.

Several cooperative research projects in the GO-Department have focussed on sheding light on the complex multi-step reaction mechanism that strongly varies with the electrocatalytic surface and reaction conditions. $H_2O_2$, a known side product or intermediate, offers the opportunity to selectively study the serial pathway, which was exploited in combined electrochemical and theoretical investigations [1,2]. The $H_2O_2$ decomposition reactions on platinum were shown to be very fast (diffusion limited) for a wide range of potentials showing that the serial ORR pathway is possible even if $H_2O_2$ cannot be detected. Electronic structure calculations of the activation energies confirmed, that reaction pathways and kinetics of the peroxide decomposition are controlled by the oxidation state of Pt surfaces (see p. 129). Surface sensitive vibrational spectroscopy allows direct detection of ORR intermediates and thereby validation of the mechanism. A spectro-electrochemical ATR-IR setup has been developed and in a first application ORR on the model semiconductor surface *n*-Ge(100) has been studied [3].

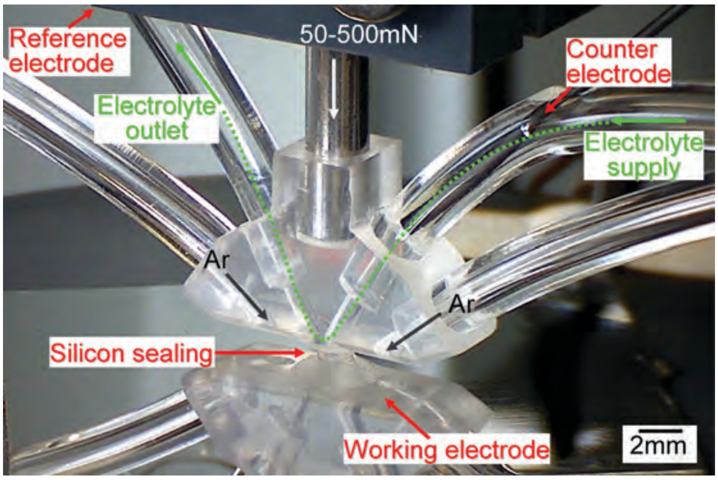


**Fig 2:** *The core of the Scanning Flow Cell is an electrochemical cell made out of polyacryl with two channels for the electrolyte inlet and outlet that are housing the reference and counter electrode. The electrolyte flow is induced by a peristaltic pump (not shown). The cell has an opening at the bottom of 200-1000 µm surrounded by a silicone sealing, which defines the contact area on the working electrode sample. The electrolyte can be purged by various inert or reactive gases; additional gas line for creating an inert atmosphere around the sealing prevents oxygen diffusion through the silicone. The whole cell is mounted on a xyz-translational stage for automatic position control, and can be operated in a free hanging mode or full contact mode with controlled contact pressure.*

Within the last years, **the newly developed and unique Scanning Flow Cell (SFC) coupled to the inductively coupled plasma mass spectrometer (ICP-MS) depicted in Fig. 2** has become a workhorse for high-throughput investigations of the stability of electrocatalysts, and the study of electrochemical processes such as corrosion or dealloying [4-6]. This has been utilized to increase the **understanding of the (electro-)chemical dissolution of metals** as a critical process for both, the design and synthesis of new catalysts and the prevention of their degradation during operation. Due to the wide parameter-space for material composition and structure as well as operation conditions fast screening techniques are necessary to obtain reliable information within a reasonable timeframe. For this purpose the scanning flow cell (SFC) automated high-throughput technique has been extended to enable the analysis of finely dispersed, porous catalyst materials. In cooperation with the industry partners the activity and stability of different catalysts for the application in polymer electrolyte membrane fuel cells has been a central aspect of the SFC work. Polymer electrolyte fuel cell technology is considered as one of the possible alternatives for electromobility applications, however the extensive use of and the degradation of Pt especially at the cathode still prevents its commercialization. Alloying with transition metals is a common strategy to generate highly active yet stable ORR electrocatalyst, as it lowers Pt loadings and also increases the activity due to ligand or strain effects. However, the instability arising from the electrochemical dissolution of the less noble metal, causing a decrease in the activity and poisoning of the membrane remains. On the other hand, dealloying before implementation in the membrane-electrode-assembly can be a useful tool in designing catalysts as it improves activity compared to conventional catalysts [7]. To follow the microstructural changes of Pt-based catalysts at a nanoscale level we employ the combination of conventional electrochemical techniques and the Identical Location TEM approach (IL-TEM – see p. 131). The latter provides insights in the dealloying pathways, size dependent morphological changes and degradation process. Extending the IL-TEM to more sophisticated characterization techniques (HAADF-STEM, EELS and tomography) allows an investigation also of the compositional variation on the sub-nanometer scale and the development of a 3D reconstruction of the particle dispersion. Combining this approach with conventional electrochemistry provides a complete description of the catalytic activity in relation with the surface structural characteristics. The scientific aim is to understand the mechanisms that govern the corrosion of the materials in order to design catalysts with high stability without compromising activity. The SFC was complementarily used to characterize the **early stage of de-alloying of model $Cu_3Au$ and $Cu_3Pt$ single crystals** for developing a fundamental understanding of dealloying processes. To keep in touch with real world applications, high-surface-area bimetallic nanoparticles like CuPt were studied in parallel. Selective leaching of less noble elements from such nanosystems results in formation of porous and/or core/shell structures preserving the increased activity towards such important reactions as electrochemical oxygen reduction.

Currently, **Li-ion batteries** are the main alternative in use as energy storage in the automotive industry and in portable consumer electronics. The anode in Li-ion batteries represents a very reactive electrode, which often requires *in-situ* measurements to address the actual mechanisms at work during charging and discharging reactions. For the use with ionic liquids we have recently adapted and now intensively tested a UHV-compatible *in-situ* electrochemical X-ray diffraction chamber employed at synchrotron light sources. By their low interaction with matter especially high-energy photons in the range above 60 keV offer great possibilities for *in-situ* diffraction studies. Eventually replacing carbonaceous materials, silicon may become one of the most important anode materials in the future. Theoretically it can store many times more Li but structural and primarily volume changes pose currently still technical problems. Au nanoparticles are one way to obtain Si nanowires but the strong Au–Li signals obscure the interpretation of X-ray diffraction data from the Si nanowires. Here we started to examine pure Au model systems [8,9] with high-energy synchrotron light at the new light source PETRA3 in Hamburg and could unambiguously identify two metastable Au-Li phases, which constitute the main phases during cycling. Further work will focus on different Si-based materials and using the new **Pulsed Laser Deposition** system for producing thin film model electrodes.

## Corrosion

The corrosion research of the department includes aqueous, atmospheric and bio-corrosion processes and their inhibition, covering both fundamental and applied aspects. In aqueous environments the SFC system with downstream analytics allows **electrochemical high-throughput screening and characterization of corrosion properties of material samples**. The setup allows the time-efficient investigation of samples by electrochemical methods (OCP measurements, potentiodynamic sweeps, galvanostatic polarization, electrochemical impedance spectroscopy, etc.) on a very small area of about 0.2 mm$^2$. The UV-VIS detector downstream of the electrode analyzes in parallel the dissolved amount of an element, and from these dissolution profiles the corrosion current density of the material can be determined directly and compared with electrochemical data. All measurements are fully automated and controlled by in-house programmed *LabView* routines and the SFC was extended as routine tool for the evaluation of corrosion properties in industry laboratories.

**Amorphous and nanocrystalline Fe-based materials** have been targeted as unique model alloys for fundamental corrosion research. The stainless-type alloy system Fe$_{65-x}$Cr$_x$Mo$_{14}$C$_{15}$B$_6$ can be reliably produced in the ultimately homogeneous amorphous state as well as, by applying specific heat treatments, in partially (to a varying extent) or fully crystallized versions. The very short length scale of the formed inhomogeneities renders these materials ideally suited for high-resolution techniques such as Atom Probe Tomography and Scanning Auger Electron Microscopy, which provide an unprecedented detail of the elemental distribution. The associated well-characterized surfaces serve as the starting point for further unique electrochemical corrosion experiments. In this respect the Scanning Flow Cell ICP-MS setup could provide simultaneous current-voltage measurements and time-resolved individual elemental dissolution behavior. By combining a unique set of experimental techniques an entire corrosion process could be thus followed from the atomic bulk structure right into the electrolyte (see p. 123).

**Stability of metal alloy surfaces and in particular dealloying reactions is another important corrosion-related topic studied in the department.** Noble metal binary alloys constitute here the main set of addressed samples. Originally such alloys were studied to understand dealloying-related stress-corrosion cracking in brass materials - nowadays the nanoporous noble metal structures that can be obtained by dealloying have direct technical applications from sensors and actuators to catalysis and batteries. Utilizing a well-studied sequence of surface structural transitions on Cu$_3$Au(111) we could gain a deeper insight in the working mechanisms of the dealloying process [10]. Further control of the surface processes and resulting morphology of the dealloyed layers could be obtained using corrosion accelerators such as halide additives and inhibitors such as plasma-polymer films or applied self-assembled thiol or selenole layers. The obtained knowledge may be very helpful in creating microstructured porosity especially for sensor applications or microreactors. In particular the thiol-modified surfaces opened up completely new views on initial cracking events and thus close back the circle to attempting to understand dealloying and stress-corrosion cracking.

Under practical application of commercial materials in most cases the underlying corrosion mechanisms are very complex, especially during **long-term exposure conditions**. That is the reason why there is up to now no accelerated test available for really reliable prediction of the corrosion performance under real practical conditions, nor a theoretical simulation tool. One key factor that will play a crucial role in determining the long term performance is the heterogeneous nature of most real life corrosion cases. In the framework of a bilateral project with TKSE and a broader set RFCS project, for instance, strong indications were found that the formation of local cathodes and anodes on the micron and submicron scale and their effect on local pH and concentration of dissolved metal cations play a decisive role for determining the protective properties of the growing corrosion product layer on the alloy, that leads to a certain degree of "passivation" of these otherwise quite reactive materials. For a real fundamental understanding of the underlying mechanisms, however, *in situ* high-resolution methods are necessary. That is why in addition to the work carried out on SECPM, an STM based potentiometric technique, as described in the last report, further methods were developed, such as a combined SECM and SKP system, that allow to perform *in situ* electrochemical investigations and *ex-situ* SKP exactly on the same area. This was at first successfully applied on dedicated aluminium model alloy samples (see [11-13]). Also first steps for the simulation of the surface pH have been carried out [14,15]. Another important project was to investigate the beneficial role of Mg cations on inhibiting oxygen reduction on cathodically polarized iron, in order to understand the reported excellent performance of zinc-magnesium alloy coatings at the cut edge or scratches down to the steel. It could be shown that the significant protective effect found at early stages is not correlated to an improved precipitation layer of corrosion products, but rather to a direct modification of the iron oxide [16].

In the understanding of the **initial stages of corrosion processes under aqueous environments**, the electronic structure of the forming corrosion products is crucial for charge and material transport and the consequent development of the corrosion reaction. A novel analysis scheme for *in situ* spectroscopic ellipsometry has been developed to enable a model-independent extraction of layer thicknesses and absorption spectrum of the forming, nm-thick layers. Results for zinc in carbonate show the presence of two different time scales in the layer growth, the formation of ZnO is decoupled from the formation of an oxidation layer [17]. Further application to copper in different media shows *in situ* the formation of oxides in different oxidation stages, depending on the conditions.

Moreover, the **electrochemical properties of the oxide layers** play a key role in the corrosion behaviour of metals and metal alloys. Within the reporting period it was investigated how different surface treatments of aluminium change the properties, especially the position of the Fermi level [18,19]. For the corrosion performance of zinc alloy coatings at the cut edge, the properties of the iron oxide on the exposed iron or steel was identified to determine the corrosion rate of the zinc alloy. Strong indications were found that zinc cations exchange with reactive $Fe^{2+}$ sites in the oxide, thus significantly inhibiting oxygen reduction. This inhibition is synergetically enhanced by the presence of magnesium cations (see [16]).

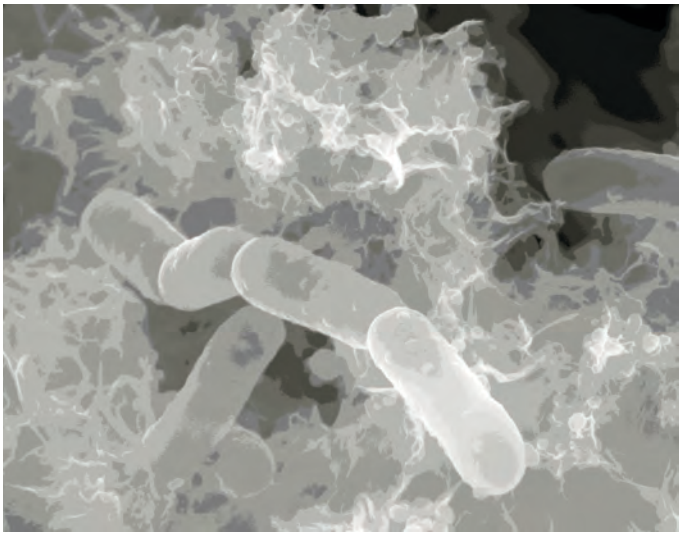


**Fig. 3:** *Sulfate-reducing bacteria (Desulfopila corrodens strain IS4) in their extracellular polymeric substance on an iron substrate causing anaerobic microbially influenced corrosion.*

**Biocorrosion** of iron that arises in anoxic environments is predominantly ascribed to anaerobic microbially influenced corrosion (MIC), with marine sulfate-reducing bacteria (SRB, see Fig. 3) being the major contributors [20]. Anaerobic MIC causes serious damages in the oil and gas industry, thus assessing and monitoring of corrosion problems and also elucidating the yet unresolved corrosion mechanism is of great importance. In close cooperation with the Max-Planck-Institute for Marine Microbiology in Bremen we work on quantifying corrosion rates *in-situ* and gaining a more detailed insight into the fundamental electron transfer mechanism at the electrode/bacteria interface. Therefore SRB strains with high corrosion activities in comparison to other well-investigated strains are studied in a multidisciplinary approach utilizing electrochemical techniques, surface analytics and molecular biological methods.

### Adhesion, thin films and friction

In **modern corrosion protection systems**, the concept of inhibitor release from capsules incorporated into metallic coatings is one important direction. Mesoporous $SiO_2$ is a well-suited material, however, its incorporation into metallic layers, *e.g.* Zn, in the electrogalvanisation process, proved to be challenging. By modification of the particles with silanethiols, the metal/oxide interface energy is modified accordingly to enable an incorporation into the growing metal [21]. Incorporation is only observed above a critical radius [22]. Besides, a thorough characterisation of genuine bifunctional silane monolayers for use as adhesion promotors on oxide-covered Si was conducted [23]. This work attracted considerable attention and was the most downloaded article in Appl. Surf. Sci. in summer 2012.

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 expertises of the department**. However, while in the past the focus was mainly on the fundamentals of delamination from plain metals such as zinc and iron, delamination from multiphase zinc alloy coatings, for instance, requires approaches with much higher resolution. For this the Scanning Kelvin Probe Force Microscope (SKP-FM) of the department was modified for dedicated *in-situ* experiments on delamination. First experiments were successfully performed on filiform corrosion and it could be shown that cathodic delamination at the head of the corrosion filaments can play a crucial role in coupling the anodic head with micron size active cathodic sites at the interface [24,25]. Another approach for better understanding is to simulate polymer/metal interfaces by preparing well defined terminations of the oxide layer and studying the effect on the properties of the resulting interface with polymers [26].

In this respect also **molecular forces at electrochemical interfaces** play a critical role in understanding and ultimately preventing adhesive bond failures in materials applications. In collaboration with the University of California at Santa Barbara (Prof. J.N. Israelachvili) we developed two newly designed experiments: the **Electrochemical Surface Forces Apparatus (EC-SFA)** [27] **and a novel electrochemical AFM** [28] **setup**, which uniquely provide *in-situ control of surface potentials and interfacial electrochemical reactions* and a simultaneous measurement of normal interaction forces, friction forces, distances and surface separations as well as contact shapes between dissimilar apposing surfaces. Using the EC-SFA setup we showed that surface morphology and in particular nanoscale roughness significantly altered the effective counterion distribution and measured force profiles at electrified interfaces. Moreover, the EC-SFA allowed for the *in-situ* structural identification and characterization of electrochemically growing (or modified) oxide thin films. In particular, the thickness of anodically growing oxide films was measured *in situ* with Å-accuracy on rough and smooth surfaces. Finally, we performed **potential dependent friction force measurements** [29] at electrode-ceramic contacts that revealed a dramatically increased shear viscosity at electrified interfaces, which is likely due to migration and redistribution of ions at the interface and restructuring of water into solid-like layers. The development of the EC-SFA tribocorrosion and in particular analysis of damage occurring under tribological conditions will further extend our portfolio in the next years. The EC-SFA provides the means to simultaneously correlate thin film rheological properties, interaction forces (adhesion and friction) and interfacial electrochemical reactions at electrified interfaces.

### Functional surface and interfaces

The development of **coatings for corrosion protection** within the department focuses mainly on the application of conducting polymers and particle modified zinc coatings. It was found that in principle three different cases exist for metal coatings based on conducting polymers: enhanced corrosion where the conducting polymer oxidises the metal and the conducting polymer in turn is re-oxidised by oxygen from the air; a passive interface with electronic contact between metal and conducting polymer, which is the targeted situation as it allows a corrosion triggered release of self-healing agents; and a situation where electronic contact between metal and conducting polymer is lost, leading to Fermi level misalignment between these two. The first and the last cases have both to be avoided. A simple SKP based screening method was developed for characterising the different coating systems in regard to these three cases and first models are proposed to explain the underlying mechanisms [30]. This will play an indispensable role for developing reliable coating systems. The storage of active substances inside the zinc (alloy) coating is considered to be of central importance for ensuring self-healing coating systems that will be fully operative even after long term exposures: the more reactive components, such as catalysts initiating polymerisation of monomers released from the organic coating, will be safely stored in the zinc (alloy) coating that is impermeable for water or oxygen. The synergy between agents stored in the zinc coating and an organic or inorganic-organic hybride coating is also the central concept of the MPG-FHG cooperative project on active corrosion protection (ASKORR) carried out together with MPIP, SIC and IAP (see report on ASKORR). One of the main problems for the storage of capsules in zinc, the difficulty to electrodeposit water dispersable capsules into zinc coatings, was successfully overcome [21].

A **molecular level understanding of interaction forces** and dynamics between *asymmetric* opposing surfaces in water plays a key role in the utilization of molecular structures for functional and smart surfaces and coatings. To quantify interaction forces and binding dynamics between opposing surfaces in terms of their chemical and molecular design we developed a novel surface forces apparatus experiment, utilizing molecularly smooth self-assembled monolayers (SAMs). Varying the SAM headgroup functionality allowed us to quantitatively identify which interaction forces dominated between the functionalized surfaces and a surface coated with a precisely controlled number density of short-chain, amine end-functionalized polyethylene-glycol (PEG) polymers. We could directly quantify and distinguish (a) specific bindings, (b) steric effects of polymer chains and, (c) adhesion of the polymer backbone, all as a function of the solution pH. Combined with novel synthetic approaches this newly developed concept will allow a very accurate molecular quantification of binding interactions between arbitrary chemical functionalities, and polymer backbones with surfaces [31].

### Industrial processes

In outdoor applications **conversion coatings** constitute a fundamental cornerstone for corrosion protection. Traditionally, phosphating is employed. Novel steel surfaces containing oxides, which cannot be attacked by pickling, are difficult to phosphate. On the other hand, passivating oxides may be relevant candidates for providing corrosion protection through grain boundaries in the phosphate coating, which would supersede the use of nickel in the baths. Using electrochemical phosphating, fully phosphate-covered surfaces on Al/Si surfaces could be obtained. Currently, their corrosion protection performance is under investigation. A new project was started on nanoceramic conversion coatings together with Henkel AG & Co. KGaA, investigating the behaviour of the future pretreatment systems under electrochemical polarisation.

Moreover, **zinc based metallic coatings** are of tremendous importance for corrosion protection and are object of research since decades. Besides others, salt spray tests have been used extensively for this purpose by applied researchers, providing however only a partial picture of corrosion processes under actual environmental conditions. The novel high-throughput screening approach based on a microelectrochemical flow cell system is able to deal with the issue of the complex interrelation between many experimental parameters, in particular the variable ion composition of salts. For this purpose the setup has been extended for fully automated switching between electrolytes while still enabling a facile coupling with downstream online analytics. In a strong collaboration with Arcelor Mittal/OCAS this is utilized first of all to increase our understanding of the impact of the electrolyte components on the fundamental corrosion mechanism and kinetics, and shall finally lead to enable tailoring of corrosion protection coatings with respect to the exposure conditions.

**Hot dip galvanising** is another industrial production step, which is intensely investigated within the department. At the focus in the last two years were co-segregation effects of alloying elements in surface oxide formation [32-34] and effects of oxygen partial pressure not only on the wetting properties of liquid zinc but also on the subsurface structure and its mechanical properties [34-36]. Especially noteworthy is the development of a **novel thermo-balance set-up** that allows measurements even during fast heating and cooling steps (see thermo-balance highlight), such as. *e.g.*, during recrystallization annealing before hot dipping. This set-up was developed within the RFCS project “HEAT” where the aim is to grow an ultra-thin iron oxide layer during soaking that serves as diffusion barrier for alloying elements.

Fundamental problems of **oxidation and hydrogen uptake during industrial production** steps of high strength steel sheet are at the focus of the Christian Doppler Laboratory of Michael Rohwerder [37-41]. Significant advances on developing a novel method for hydrogen detection based on SKP were made (see p. 119) [39]. Further, the thermodynamic simulation tool developed within the CD lab (see p. 137) was applied to different key isssues. Hydrogen uptake during high temperature production steps, such as, *e.g.*, recrystallization annealing was investigated in detail. Based on *ex-situ* [42] and *in-situ* (ambient ESCA performed at BESSY) analytical investigations we could show that the hydrogen uptake is correlated to the effective oxygen coverage of the surface and that some alloying elements such as Mn can decrease the water dissociation reaction, which results in lower oxygen coverage and higher hydrogen uptake.

## Scientific Groups

### Electrocatalysis (Karl 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.

Technically, the group is developing new electrochemical methods to investigate model and applied electrode materials. High-throughput combinatorial screening tools combined with sophisticated automation and synchronization of the experimental setup (see Fig. 2), as well as advanced methods for data evaluation and processing play thereby a major role [43]. This enables investigation of a large number of samples more systematically and reliably in shorter time. In addition, coupling electrochemistry with online reaction product determination by Inductively Coupled Plasma Mass Spectrometry [4,5] and Differential Electrochemical Mass Spectrometry (DEMS, see p. 18) increases the information depth significantly.

Besides these technical advancements, we are interested in various topics in electrocatalysis that we address with our advanced techniques. Together with the group of A. Auer we are investigating the $H_2O_2$ reactions as an important intermediate in the oxygen reduction reaction (see p. 129) [1,2]. Other important aspects in our research are the influence of the surface pH [14,15] and the effect of the electric double layer on the adsorption of reaction intermediates and the reaction kinetics itself. The latter becomes especially important when considering the effects that determine the activity of supported nanoparticle catalysts or de-alloyed, porous catalysts, since they behave quite different from extended surfaces [44,45]. $CO_2$ utilization by electrochemical means for the production of so-called solar fuels is a further hot topic in our group related to energy conversion and storage, and will be investigated in our new laboratory (p. 18) [46].

The conditions during these reactions at the solid-liquid interface are often quite harsh and lead to corrosion of the electrode material. Therefore, particular research focus in our group is placed on fundamental and applied aspects of stability. We investigate online, and in parallel to the activity, the dissolution of elements under different experimental conditions to derive the determining steps in the mechanism, and quantify the individual element contribution to the overall dissolution. This is not only of high value for noble electrocatalyst materials based on Pt or Rh, but is also of great importance for complex materials like steels (see p. 123), ZnO for photovoltaic applications [47,48] or protective coatings based on Zn/Mg/Al. Moreover, utilizing our Identical Location – Transmission Electron Microscopy approach we study the degradation of high surface area catalysts as well as de-alloying phenomena and porosity formation on the nanoscale (see p. 131) [49,50]. In collaboration with the Max-Planck-Institut für Marine Mikrobiologie in Bremen we investigate the anaerobic corrosion of iron and steel by sulfate reducing bacteria (see Fig. 2).

### Atomistic Modelling (Alexander A. Auer)

Atomistic modelling of electrochemical processes, interfacial properties and novel materials are central aspects in the work of the atomistic modelling group. Besides on-going method development in the field of post-HF *ab initio* method [51] computational studies in close collaboration with experimentalists yield insight into complex phenomena, as simulations can be used to complement experimental results from surface science and spectroscopy.

One example for this is the work on the oxygen reduction reaction on various substrates like Pt nanoparticles (see highlight ORR). The segregation behaviour of Platinum Cobalt core shell particles had been investigated previously by Mayrhofer et al., who found that Co-core Pt-shell particles can be obtained by CO annealing and that upon electrochemical treatment in the ORR the lesser noble metal is leached out. A theoretical investigation was carried out on a Pt-NP model system in which favourable and less favourable Co-substitution sites were identified. Furthermore, the influence of Oxygen and CO on the segregation energies were investigated [52]. The results do not only confirm experimental findings but also yield insight into a stepwise segregation mechanism in which the fact that NPs are fairly ductile systems plays an important role.

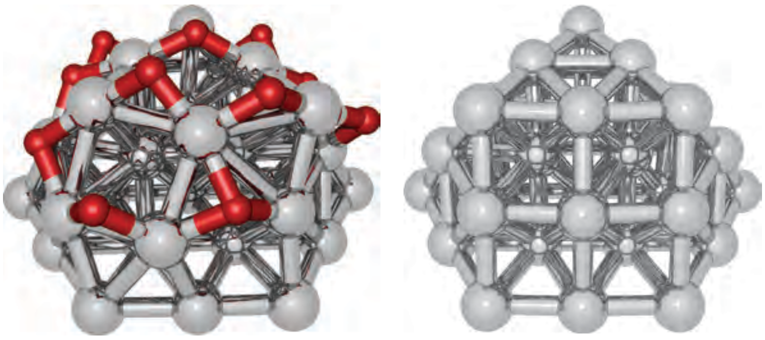


**Fig.4:** *Ductile system: Pt37 model system exhibits the properties of small nanoparticles, upon oxygen adsorption significant distortion of the system occurs.*

DFT calculations using nanoparticle-models prove to be very versatile as they can be used to investigate intermediates of the ORR as well as material properties of real catalysts (see Fig. 4). In further investigations fundamental questions have been studied concerning schemes to model the electrochemical potential for nanoparticle systems [53]. Theoretical approaches to describe electrochemical processes including the influence of the solvent and electrode potential have been further developed and applied to the ORR mechanism at highly active metal catalysts as well semiconducting interfaces.

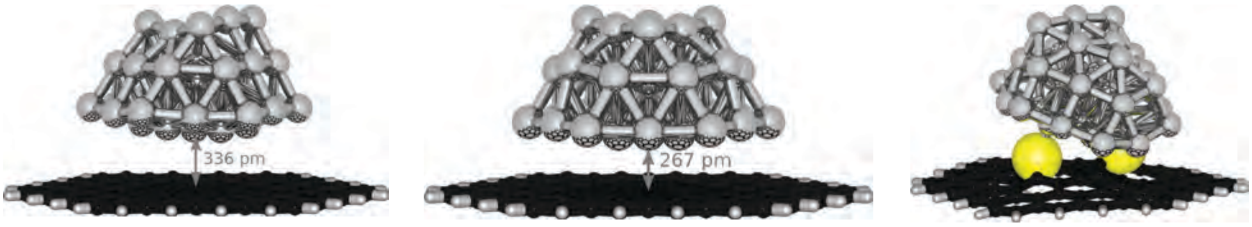


**Fig. 5**. *Interaction of the Pt37 cluster with a graphitic carbon support model – classical DFT result (left), DFT-D with inclusion of dispersion correction (center) and with sulphur as linking unit (right). As the linker also acts as a spacer, reducing the dispersion interaction, the adhesion is actually decreased in this case.*

Furthermore, problems in the application of NPs, which often are used in conjunction with carbon support, have been investigated (see Fig. 5). A computational study of the metal-carbon interaction shows that it is not only vital to apply state-of-the art dispersion interaction corrected DFT approaches but also that the main bonding mechanism is based on weak interactions with the support. For experimentalists this work yields insight into the basic adhesion mechanisms and how functionalization of the support can be carried out to improve the adhesion of the particles [54].

Extending previous work on the ZnO(0001)/water interface a Ph.D. Thesis has been launched to characterize the non-polar ZnO(10-10) and (1120) surfaces as well as the polar ZnO(000-1) surface interacting with water in order to gain a complete picture of the surface properties of this important material in corrosion protection, and catalysis under in-operando conditions as basis for future adhesion and corrosion studies. Building on the acquired expertise on ZnO surfaces, the ORR mechanism on ZnO(10-10) has been analyzed using a cluster model for the interface. Comparison to the mechanism in homogeneous solution allows to quantify the electrocatalytic properties of this surface.

In the framework of the Forschergruppe 1497 “Zwillingspolymerisation von Organisch-Anorganischen Hybridmonomeren zu Nanokompositen” a series of investigations has been carried out in order to understand the basic mechanism of the twin polymerisation [55]. This novel technique allows to synthesize inorganic/organic hybrid materials with domain sizes in the range of a few nanometers. This reaction has been intensively investigated during the last years from which $SiO_2$/Phenol resin nanocomposites, for example, can be obtained in a single step synthesis from one type of monomer. Novel approaches using Ga or Ge oxides as inorganic component might open the route to materials with high potential for application in various fields [56].

The very fruitful collaboration with the group of Prof. K. Banert from the organic synthesis group at the TU Chemnitz has lead to a series of successful projects focusing on the synthesis of novel compounds that have witnessed quite some interest in the literature. These have been published with title pages in *Chemistry - A European Journal* in 2011 and in *Angewandte Chemie* in early 2012 [57,58] and demonstrate the versatility of applications for accurate electronic structure calculation (see Fig. 6).

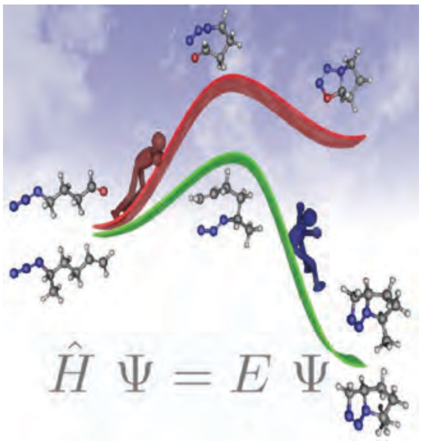


**Fig. 6:** *Accurate ab initio calculations reveal possible reaction paths and can help to guide experiments as well as correct synthesis for which products have been misinterpreted.*

In collaboration with Bayer Leverkusen and ICAMS multiscale modelling techniques have been developed to simulate the network formation and mesoscale structure formation processes during the curing of polyuretanes. A detailed coarse-grained (mesoscale) simulation including accurate conformational and intermolecular interactions as well as reactivity was developed based on DFT and atomistic force-field calculations and calibrated against available experimental data. Future work will also include the reactivity at, *e.g.*, ZnO surfaces and interphase formation to better understand adhesion and to develop an atomistic interface model for studies of mechanical properties, reactivity with environmental agents, deadhesion, and corrosion.

### Interface Spectroscopy (Andreas Erbe)

The Interface Spectroscopy Group continues to work in two different directions, (1) the design of interfaces for spectroscopic investigations with their application to the study of electrochemical reaction mechanisms and (2) chemical modification of material's interfaces to tailor surface properties and to investigate failure mechanisms.

The theoretical optical part has progressed the understanding of infrared spectroscopic experiments from rough interfaces [59,60]. Using finite element solutions of the Maxwell equations, details emerge which regions of an interface with complex morphology are actually accessible to light [60]. Transparency of thin continuous metal films was enhanced through the application of anti-reflection coatings on the metal [61]. A further improvement of the scope of infrared spectroscopy at interfaces can be achieved through the use of intense tunable laser light sources. A first step in our lab was the establishment of a reflection setup involving a pulsed, tunable quantum cascade laser [62].

In the ultraviolet and visible spectral range, spectroscopic ellipsometry was used to study the evolution of oxide on zinc *in situ* (see p. 133) [17,63]. Both in oxygen-containing and oxygen-free atmospheres [63], as well as in electrolyte [17], the evolution of the layer thickness is decoupled from the evolution of the electronic structure of the layer. The electronic structure is probed through the absorption spectrum at photon energies between 1 and 4 eV.

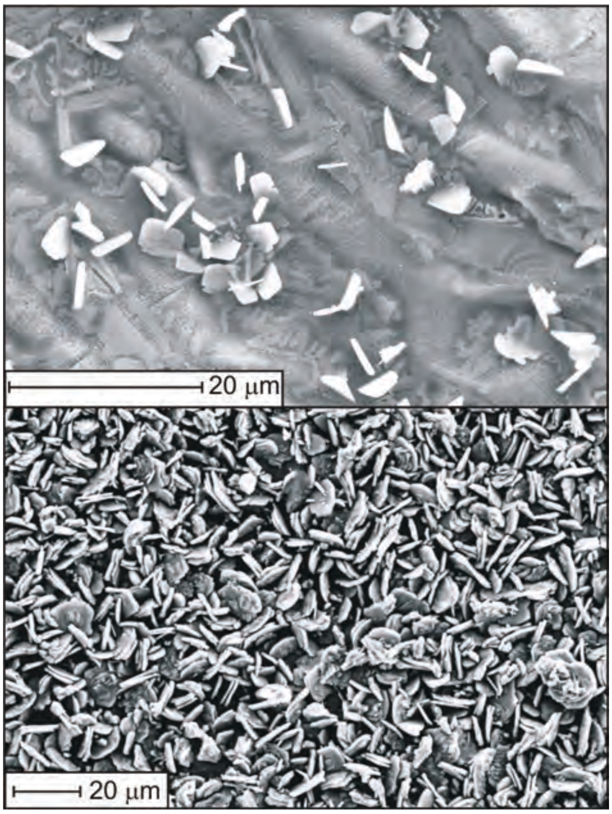


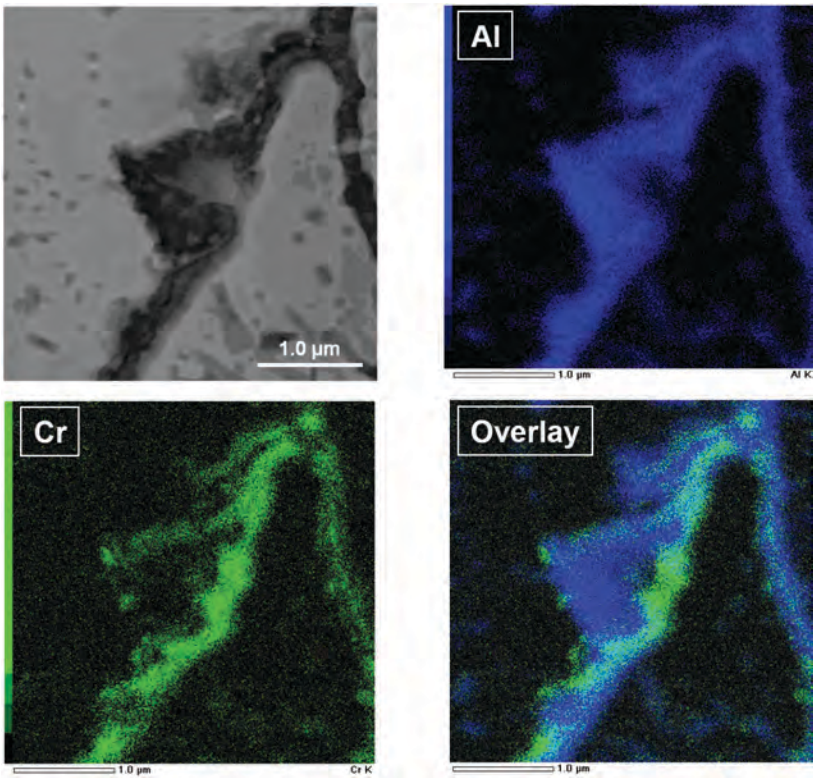
**Fig. 7:** *Two different stages of the phosphating process of AS steel.*

A collaboration was established with the group of Patrick Koelsch, formerly at Karlsruhe Institute of Technology, now at University of Washington, Seattle, who is an expert in modern vibrational sum-frequency-generation (SFG) spectroscopy. Complemented by ellipsometric analysis at MPIE, femtosecond-broadband SFG spectroscopy was applied to electrochemically highly stable araliphatic self-assembled monolayers (SAMs), which was studied extensively in the group "Molecular Structure and Surface Modification" [64,65]. The SFG results show on the one hand the surprising maintenance of ordered structures after electrochemical desorption of the SAMs [64]. The detection of a mixing of the static electric field with the SFG signals may enable a direct access to the interfacial electric field in the future [65]. Details of these results are presented as a highlight in this report. A collaboration with the Institute of Physics, Academia Sinica, Taiwan, resulted in the fabrication of a ~5 nm wide gap between tip metal electrodes, which have been used to trap protein molecules for Raman spectroscopic studies [66]. In the future, such devices will enable electrochemical experiments with ultralow sample amounts.

On the chemical surface modification side, in collaboration with industrial partners, work on conversion coatings is performed. An electrochemical, fluoride free process was developed to enable phosphating of oxide-covered Al/Si metallic coatings (Fig. 7). In a new project, properties of modern conversion coatings under the application of electric fields are investigated. Electrocatalytic properties of gold towards methanol oxidation were studied, and a method based on lead deposition used to remove organic material from the electrode surface [67]. While adhesion promoters on silane-basis are long known in industry, their adsorption often results in ill-defined multilayer structures. Systematic investigations of the adsorption resulted in the establishment of a protocol to form well-defined monolayers, which were thoroughly characterised [23]. Such structures are currently being exploited for molecularly defined anchoring of polymer coatings on oxidic surfaces. In cooperation with Max Plank India Fellow Pritam Deb of Tezpur University, a central university in India, chemical surface modification with organic materials of different iron oxide particles was and still is investigated [68].

In a new project within the framework of the Marie Curie Initial Training Network (ITN) "Somatai", diffusion in novel water-based coatings will be investigated. Somatai will be a new opportunity to link our activities to partners from the soft matter community. The understanding of polymer-based coatings will certainly benefit from this project. As the Somatai website will be hosted at MPIE, we will be involved in the ITN at a central position.

In addition, we provide support to the institute in application of optical characterisation techniques, and with know-how on the properties of light. An important example is the optical characterisation of biological photonic structures in collaboration with the Department of Microstructure Physics and Alloy Design (see p. 139).



**Fig, 8:** *Layered structure of a grain boundary oxide: EDX elemental maps of a FIB-prepared TEM (cross-sectional) lamella of ternary Fe−3Al−0.8Cr model alloy annealed at 700 °C, in* $N_2$*/2.5%*$H_2$*/9000ppm*$H_2O$*, for 2 hours.*

### Christian Doppler Laboratory for Diffusion and Segregation during Production of High Strength Steel Sheet (Michael Rohwerder)

The main focus of this lab is on fundamental diffusion and segregation problems encountered during the different production steps of high strength steel sheet. Cooperation partners are voestalpine and TU Wien.

The technical motivation behind this is 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 is 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 in three 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 (see Fig 8) and developing a new simulation tool for describing grain-boundary oxidation on a theoretical level [39-41]. One important result found within the reporting period was that it is mainly the interaction between some of the key alloying elements in high strength steels that is responsible for significantly enhanced internal oxidation. This is at the focus of current research and will be investigated experimentally and theoretically.

**P (Pickling) Module:**

This module deals with pickling after hot rolling and is carried out mainly at the TU Wien (Prof. Danninger).

**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 latter an important question is information about the distribution of oxides at the different stages of the annealing [42], which is now also investigated by ambient ESCA. Here a main focus in the reporting period was the successful development of a novel method for spatially resolved highly sensitive hydrogen detection (see p. 119 and [37,38]).

### Molecular Structures and Surface Design (Michael Rohwerder)

The main scope of this group is to address fundamental questions of surface and coating technology by isolating the crucial problems behind them and designing model experiments and model samples for their systematic investigation. A technique of central importance for many research projects within the group is the Scanning Kelvin Probe technique. Based on the world leading expertise in this technique also novel application fields are explored.

The correlated main activities on these research interests 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 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. In cooperation with Prof. Wöll (KIT) and Prof. Terfort (Univ. of Frankfurt) our investigations on oxygen reduction at self-assembled thiol monolayer films are extended on a broader base of various aromatic thiol molecules. In order to establish the targeted structure-reaction correlation on the molecular and nanoscopic scale a thorough characterisation of the monolayers is carried out [69,70].

The investigations on monolayer stability provided also extremely interesting results on hydrogen evolution at organic layers and on metallization of self-assembled films. The hydrogen evolution reaction seems to be enhanced at the first stages of cathodic monolayer desorption, which is due to the prevailing molecular order of the film directly after desorption (see p. 135).

Side results of this work were the development of a novel approach for optimizing the complexation of metal cations on self-assembled monolayers and their electro-less reduction by hydrogen (see highlight report), which provides metal monolayers of superior properties [71,72]. The effect of different pre-treatments on the interface with different coatings was studied in detail for aluminium [26]. SKPFM was very successfully applied on filiform corrosion and it could be shown by performing the experiment under repetitive gas change conditions (between air and nitrogen) that cathodic delamination at the head of the corrosion filaments can play a crucial role in coupling the anodic head with micron size active cathodic sites at the interface [24,25].

### *2. Semiconducting properties of surface oxide films*

The Kelvin probe technique directly provides information about the work function of the surface oxide, which can be interpreted also as electrode potential. In how far predictions about the possible localised corrosion behaviour in a corrosive environment may be made from potential maps obtained by SKP in air is the topic of a joined project with Prof. Schuhmann (RUB), where SKP and SECM (Scanning Electrochemical Microscopy) could already be successfully combined [12,13]. This enables application of the SECM exactly on the same features as mapped by SKP. This technique was first applied to aluminium alloys [11]. Further it was investigated how different pretreatments, such as alkaline and acidic cleaning, change the semiconducting properties of the alumina layer. A strong correlation between OH fraction and Fermi level position in the oxide was found [18,19].

Another important topic are novel Zinc-Aluminium-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. However, the exact reasons are still not known. In the reporting period strong indications were found that the microstructure induced by alloying with magnesium may play a crucial role here, as it determines the lateral distribution of cathodic and anodic sites and hence the local pH, which in turm will have an effect on the growth of the corrosion product layer. Hence, prediction of surface pH is very important and first steps were undertaken [14]. The most important finding of the latest activities, however, was that at the cut edge or at defects down to the steel, the beneficial effect of magnesium at least at the initial stages of exposure is mainly due to enhancing the effect of the zinc cations, which were found to replace reactive $Fe^{2+}$ sites in the iron oxide layer and thus significantly decrease the oxygen reduction rate [16].

### *3. Wetting and interfacial reactions at metal/metal melt interfaces and selective oxidation:*

Our research on the reactive wetting behaviour of liquid zinc on a variety of steels and model alloys has provided new insight into the wetting kinetics and how it depends on oxide morphology. At the focus in the last two years were co-segregation effects of alloying elements in surface oxide formation [32-34] and effects of oxygen partial pressure not only on the wetting properties of liquid zinc but also on the subsurface structure and its mechanical properties [34-36]. A big success was the development of a novel thermo-balance set-up, where the reaction gas atmosphere is adjusted without carrier gas and thus works under sub-atmospheric pressures but with the same dew points and hydrogen partial pressures as applied in standard experiments. That allows measurements even during fast heating and cooling steps, such as, *e.g.*, during recrystallization annealing before hot dipping, without buoyancy forces and with nearly no disturbances at all (see p. 137). This setup was developed within the RFCS project “HEAT” where the aim is to grow an ultra-thin iron oxide layer during soaking that serves as diffusion barrier for alloying elements.

### *4. Intelligent self-healing concepts for corrosion protection*

The main activities on self-healing are carried out in two projects: a DFG SPP (“Self-Healing Materials”) and a MPG-FHG cooperative project on active corrosion protection (ASKORR). While the first is mainly focused on conducting polymers, the latter is set to synergistically combine capsule loaded zinc coatings with capsule loaded organic coatings for superior intelligent self-healing. Currently the main activity in the first project is on getting conducting polymers work on zinc, where conducting polymers were shown to be usually de-activated [30]. In ASKORR, after solving key issues of particle co-deposition during electrogalvanising [21], the main focus is now on realizing optimized self-healing by a synergetic inter-play of zinc and organic coating (see p. 127).

### *5. SKP as a tool for general application for processes at buried interfaces*

Besides using the SKP technique for *in-situ* investigations in synchrotron set-ups [73], also spatially resolved high-sensitivity hydrogen detection by Kelvin probe is investigated (see p. 63 (CDL lab) and p. 119).

## Interface Structures and High Temperature Reactions (Frank U. Renner)

The research activities within the „Interface Structures and High-Temperature Reactions“ group focus on utilizing high-resolution structural techniques and aim at gaining mechanistic insight in processes, possibly on the atomic scale. Staring form a surface science approach the group activities aim to bridge the complexity gap and pressure gap towards more realistic conditions of processes. This goal is achieved by studying still simplistic surfaces but in realistic environments such as electrolytes or corrosive gas atmospheres. In this line ideally ordered, single-element or (binary) alloy single-crystal surfaces but also systems such as complex, ideally disordered, *i.e.* homogeneously amorphous alloys are studied. Especially beneficial are in this context *in-situ* X-ray diffraction techniques using Synchrotron radiation, but also techniques such as Scanning Auger Electron Microscopy (SAEM) or Atom Probe Tomography. In particular the structural aspects accessed by *in-situ* X-ray diffraction are a valuable complementary addition to the department’s activities on electrochemical processes. Thus, although working on a broad scope of different subjects from oxide scale formation to Li-ion battery interfaces, the group’s main activities can be summarized as:

1. Using simplified (solid) model substrate systems such as single crystals, thin films, or amorphous/nanocrystalline materials.
2. Employing high-resolution structural techniques such as in-house lab-based Auger Microscopy as well as Synchrotron-based large scale facilities - and possibly *in-situ* studies.
3. The main interest is in the behavior of systems in real atmospheres. In the focus are electrochemical interfaces and solid-gas reactions at elevated temperature.

Dealloying is a specific corrosion process and of large fundamental relevance in other electrochemical processes such as catalysis, too. In particular the binary alloy surface $Cu_3Au(111)$ with its very particular sequence of initial structural states [10,74,75] has been used within the group’s research program as a reference system to address the influence of corrosion accelerators [28,76,77] and of inhibition mechanisms [10,28]. Single crystal surfaces modified by self-assembled thiol monolayer films revealed a distinctive cracking failure mechanism with clear crystallographic crack openings, which opened a possibility to actually address the initial stages of crack formation in collaboration with other departments (see, *e.g.*, p. 125). As dealloying of noble metal alloys was also studied early-on in the context of stress corrosion cracking these results bear a large promise for furthering understanding in an ultimately technological context.

With corrosion of amorphous and nanocrystalline steels a further promising research topic could be established. Selective dissolution phenomena in the context of passivity and wet corrosion could be in great detail related to the respective nanostructured materials in collaborations with the Electrocatalysis group (Dr. K.J.J. Mayrhofer) and the Atom Probe Tomography group (Dr. P.-P.Choi, Department of Microstructure Physics and Metal Forming). This approach of using a unique set of complementary methods bears a great potential to actually gain deeper well-characterized insight into the microstructure-performance relation of corrosion reactions and passivity.

Next to further electrochemical reactions such as electrodeposition from ionic liquids (in collaboration with Dr. M. Rohwerder), phosphating (in collaboration with Dr. A. Erbe), or battery processes (see p. 29) also elevated and high-temperature gas corrosion is studied in part with industrial partners in various

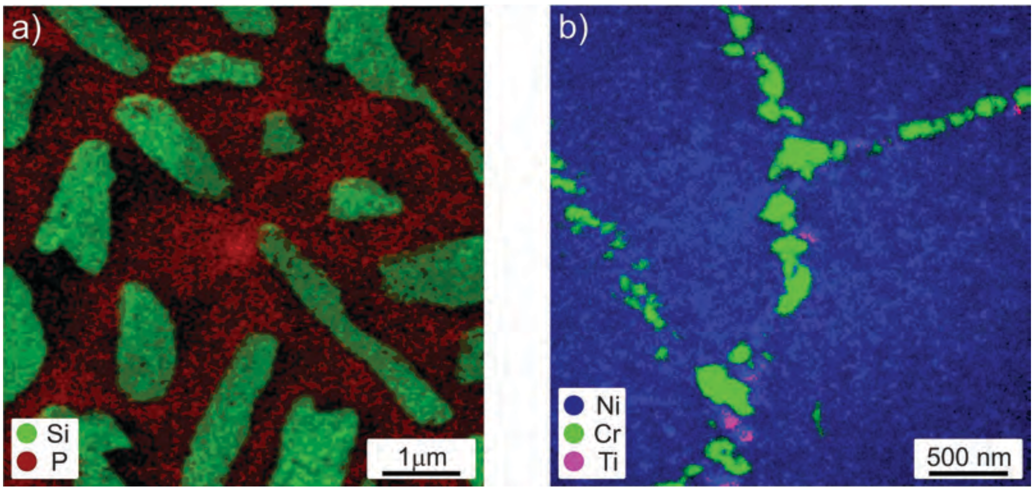


**Fig. 9.** *Scanning Auger Electron Microscopy maps of a) phosphate coverage on an AS-steel surface and b) grain boundary in a Ni-based superalloy.*

atmospheres, *i.e.* oxidation, steam corrosion, or sulphidation. These works will be continued using more high-resolution methods and *in-situ* diffraction to study the initial stages of similar processes. Fig. 9 includes two SAEM images showing the selective phosphate reaction on AS steel and a grain boundary prior to sulphidation.

### Interaction Forces and Functional Materials (Markus Valtiner)

The research interest and philosophy of the newly established group (www.mpie.de/ifor) is focused on the broad areas of adhesion, friction and interfacial forces, as well as their concerted utilization for making novel smart and hierarchically structured materials, interfaces and thin films for application in structural and functional materials. Our scientific aim is to gain insight into the fundamental interactions of complex interfacial processes, and to translate fundamental science into knowledge-based design of better and novel structural and functional materials for technological applications. We are in particular interested in:

1. Fundamental work on interfacial forces, interfacial structures and tribology under (electrochemically active) variable environmental conditions.
2. The effect of (electro-)chemical reactions on interfacial interactions with a particular focus on structural effects in confined spaces and complex environments (high salt concentrations and non-aqueous electrolytes).
3. Electrochemistry in confined spaces.
4. Measurement, understanding and ultimately prediction of properties of surfaces, interfaces and thin films over large length and time scales.
5. Design and utilization of model experiments and tunable thin films and interfaces using unique bio-mimetic and molecular design concepts.
6. Development and establishment of new experimental techniques for surface and interface analysis.
7. Preparation and characterization of advanced functional materials with smart properties.

The technological focus of the group is the *design of novel experiments and experimental setups* dedicated to understanding interfacial dynamics such as specific and non-specific binding and unbinding events at the single molecular and macroscopic level. The newly developed electrochemical Surface Forces Apparatus provides the means to experimentally realize confined environments on the sub-nanometer scale. This capability will be extended to study electrochemical reactivity and kinetics in confined spaces. On p. 16, the scientific philosophy of the group and the newly designed EC-SFA are detailed.

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## Research Projects in Progress

**Electrocatalysis** (K.J.J. Mayrhofer)

*Baldizzone:* Degradation of carbon-supported Pt bimetallic nanoparticles

*Beese, Widdel*: Anaerobic microbially influenced corrosion of iron

*Cherevko, Zeradjanin, Fink*: High-throughput material screening for electrochemical $CO_2$ reduction

*Cherevko*: Mechanism of electrochemical gold dissolution in acidic media

*Cherevko, Topalov, Ankah, Renner:* Metal dissolution during electrochemical dealloying: the case of $Cu_3Au(111)$ model system

*Hamou, Biedermann, Arenz:* EDL influence on reaction kinetics on nanoparticle catalysts

*Jeyabharathi, Hodnik:* Particle-size dependent dealloying

*Katsounaros:* Oxygen reduction reaction on noble metal catalysts

*Katsounaros,* Schneider, Auer: Understanding the mechanism of the oxygen reduction reaction

*Laska:* Effect of variable electrolyte composition on zinc corrosion investigated by a SFC system with dynamic electrolyte change

*Meier:* Study of particle size effect on fuel cell catalyst stability under simulated start up/ shut down conditions

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

*Meier, Auinger, Katsounaros:* Effect of surface pH on the oxygen reduction reaction (ORR) in neutral electrolytes

*Meier, Galeano, Schüth:* Influence of intrinsic N-doping on activity and stabilty of hollow graphitic sphere based platinum nanoparticles

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

*Schuppert:* Screening of high-surface-area catalysts for application in polymer electrolyte membrane fuel cells with the SFC setup

*Schuppert, Topalov:* Activity and stability of PtCu-alloys by screening of thin-film material libraries

*Topalov:* Stability investigation of Pt and Pt-based alloys utilizing a high-throughput SFC coupled with ICP-MS

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

**Atomistic Modelling** (A.A. Auer)

*Auer, Schneider, Benedikt*: Computational study of precious metal nanoparticle – carbon support interactions

*Auer, Schneider, Benedikt*: Computational study of the oxygen reduction reaction on Pt and Pt alloy nanoparticles

*Auer, Schneider, Benedikt*: Model development for describing electrochemical reactions on nanoparticles using quantum chemical methods

*Auer, Schneider, Benedikt*: Modelling the influence of solvent in electronic structure calculations of electrochemical reactions

*Berezkin, Biedermann (in cooperation with ICAMS and Bayer Leverkusen)*: Multi-scale simulation of polyuretane curing and interphase formation on ZnO substrates

*Biedermann*: ORR at the ZnO/water interface

*Biedermann, Bashir, Rohwerder*: DFT simulations of vibrational spectra of SAM molecules

*Biedermann, Nayak, Erbe*: Intermediates of the ORR on germanium

*Chakraborty, Auer, Biedermann, Nayak, Erbe (in cooperiation with Rochus Schmidt, RUB)*: Ge/electrolyte interface structure in function of the electrode potential

*Hamou, Biedermann, Mayrhofer*: The effect of roughness and porosity on the electric double layer and ORR catalysis

*Kenmoe, Biedermann*: DFT study of the ZnO/water inferface

*Salgin, Hamou, Rohwerder*: Application of the scanning Kelvin probe for monitoring ionic surface migration

**Interface Spectroscopy Group** (A. Erbe)

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

*Deb, Ebbinghaus, Schneider, Kostka, Erbe:* Characterization and surface modification of iron oxide nanoparticles

*Ebbinghaus, Lesser-Rojas, Chou, Erbe*: Raman spectroscopy at nanoelectrodes

*Iqbal, Muhler, Erbe*: Preparation of molecularly-defined polymer/metal interfaces and their delamination behaviour

*Iqbal, Erbe*: Nanostructuring through corrosion

*Iqbal, Bashir, Rohwerder, Erbe*: Photoswitchable self-assembled monolayers

*Moirangthem, Schwenzfeier, Erbe:* Surface water and water surfaces studied by infrared ellipsometry

*Nayak, Biedermann, Stratmann, Erbe:* Detection of intermediates in the oxygen reduction reaction on semiconductor electrodes

*Nayak, Sriram, Chou, Erbe*: Behaviour of water in confined environments

*Pengel, Stratmann, Erbe*: Time-resolved infrared spectroelectrochemistry

*Sarfraz, Posner, Erbe*: Effect of the cathodic electrodeposition coating on nanoceramic conversion coatings

*Schneider, Renner, Erbe:* Initial stages of crystallization of phosphates on the surfaces of zinc and modern steels

*Seemayer, Schneider, Renner, Todorova, Erbe:* Corrosion of iron in $H_2S$-containing sour acid media

**Christian Doppler Laboratory for Diffusion and Segregation during Production of High Strength Steel Sheet** (M. Rohwerder)

*Auinger, Rohwerder:* Simulation of selective oxidation and grain boundary oxidation

*Borodin, Rohwerder:* Investigation of hydrogen uptake kinetics during recrystallisation annealing

*Evers, Borodin, Rohwerder*: Spatially resolved and ultra-sensitive hydrogen detection in steels and investigation of hydrogen uptake

*Auinger, Swaminathan, Borodin, Rohwerder*: Fundamental investigation of grain boundary oxidation

**Molecular Structures and Surface Design** (M. Rohwerder)

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

*Ankah, Renner, Rohwerder:* Fundamental investigations of de-alloying

*Bashir, Krieg, Rohwerder:* Characterization of zinc alloys for automotive application

*Bashir, Rohwerder*: STM, SECPM and SKP for surface characterisation

*Iqbal, Bashir, Rohwerder, Erbe*: Photoswitchable self-assembled monolayers

*Krieg, Borissov, Rohwerder*: Investigation of cathodic self-healing at cut-edge, blank corrosion of ZAMs

*Liu, Swaminathan, Rohwerder*: Fundamental investigation of hot dip galvanizing

*Merzlikin, Rohwerder*: Characterisation of hydrogen in steels

*Muglali, Erbe, Rohwerder:* Oxygen reduction, hydrogen evolution and metal deposition at self-assembled monolayer/gold interfaces

*NN, Rohwerder*: Novel corrosion protection coatings for hot forming

*NN, Rohwerder*: Guidelines for use of welded stainless steel in corrosive environments

*Padhy, Erbe, Rohwerder:* Electronic structure of native oxides in dependence on the atmosphere

*Salgin, Rohwerder:* Mobility along interfaces and on surfaces and effect of modification

*Senöz, Bashir, Rohwerder:* SKPFM for the investigation of localised corrosion

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

*A. Vogel, Merzlikin, Rohwerder:* Nano-particular iron oxide films for improved wettability

*Vogel, Schönberger, Rohwerder*: QCM for high temperature application

*Vogel, Merzlikin, Rohwerder*: High emissivity annealing technique for improved hot dip galvanising

*Vimalanandan, Rohwerder:* Intelligent corrosion protection coatings by conducting polymers

**Interface Structures and High Temperature Reactions** (F.U. Renner)

*Ankah, Ma, Raabe, Cherevko, Mayrhofer, Rohwerder, Renner:* Dealloying of Cu−Au alloys.

*Ankah, Renner:* Dealloying of Cu-Pd alloys.

*Bach, Seemayer, Renner:* Advanced characterization of Li-ion battery electrodes

*Bashir, Ankah, Klemm, Valtiner, Renner (in collaboration with M.Valtiner):* In-situ AFM studies of selective inhibition by thiol u-contact printing

*Duarte, Kostka, Choi, Raabe, Renner:* Bulk segregation in heat treated amorphous steels

*Duarte, Renner:* In-situ high-energy X-ray diffraction of crystallization of amorphous steel

*Izzuddin, Renner:* Sulphidation of Ni−Al alloys

*Klemm, Duarte, Mayrhofer, Renner:* Element-resolved corrosion studies

*Lange, Rohwerder, Renner:* Grain boundary sulphidation of Ni-based alloys

*Lymperakis, Neugebauer, Renner (in collaboration with CM-Department):* Atomistic simulations of a Au/Cu−Au heterophase interface

*Madinehei, Duarte, Klemm, Crespo, Renner (in collaboration with BarcelonaTech, Spain):* Production and corrosion of low-Cr amorphous steel.

*Schneider, Lange, Erbe, Renner: (in collaboration with A. Erbe):* Surface analysis of initial stages of phosphating reactions

*Seemayer, Bach, Renner:* Model systems for Li-ion batteries

*Vogel, Palm, Renner:* High-temperature corrosion of iron aluminides in steam

**Interaction forces and functional materials** (M. Valtiner)

*Valtiner:* Unravelling of structure/property relationships at electrified interfaces

*Baimpos, NN, Valtiner*: Electric double layer structures is highly concentrated electrolytes

*Baimpos, Valtiner:* Development of novel molecular force sensors

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

*Raman, Stock, Valtiner*: Single molecule physics at electrified interfaces

# Department of Microstructure Physics and Alloy Design

*D. Raabe*

## Scientific Concept

We conduct basic research on the relationship between synthesis, structure and properties of materials, Fig. 1. The focus lies on nanostructured engineering alloys based on iron [1], magnesium [2,3], titanium [4], nickel [5,6], and intermetallics [7] as well as on biological [8] and metal-based composites [9]. Recently, also interfaces in semiconductors are studied [10-13]. These materials and their mechanical properties are characterized by complex phase transformations [14] and defect substructures [15]. To study these phenomena and their interplay we develop advanced characterization methods from the single atom level [1,14] up to the macroscopic scale and apply them together with scale-matching multiscale models, Fig. 2 [16]. Examples of experimental tools are local electrode atom probe tomography [1,14,17], 3D EBSD (Electron Back Scattering Diffraction) [18-20], ECCI (Electron Channeling Contrast Imaging) [15,21,22], and micromechanical experiments under well-controlled boundary conditions [23-28].

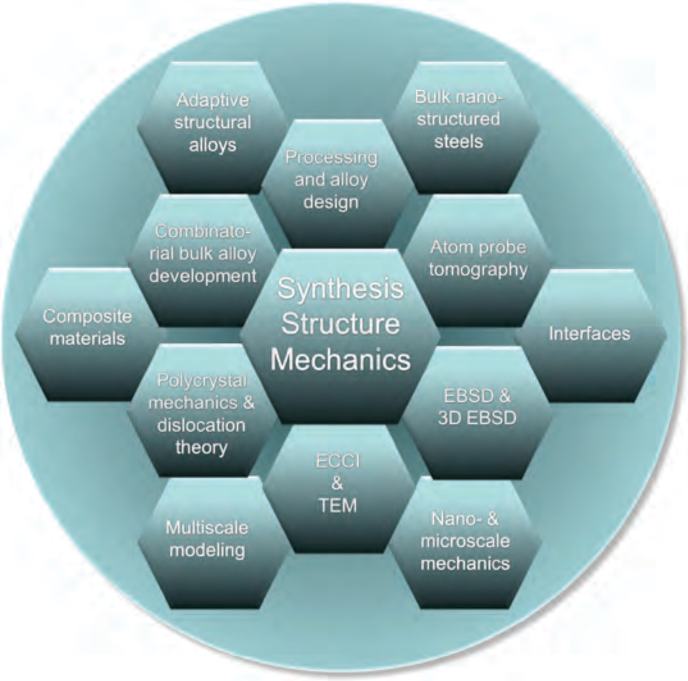


**Fig. 1:** *Main research areas in the department.*

Examples of simulation tools are defect-based constitutive models of microstructure evolution and microstructure-property relations at different length scales such as crystal plasticity spectral and finite element solvers [16,23,25,26,28-34] or discrete dislocation dynamics [35,36]. Close interfacing of simulation and experiment with the aim to quantitatively compare the two has high priority [4,8,16]. Since microstructures of engineering alloys are typically designed by imposing a sequence of thermo-mechanical treatments, the effects of synthesis and processing on the microstructure evolution and hence on the mechanical response of the materials increasingly gains momentum in our projects. Examples are the development of a new class

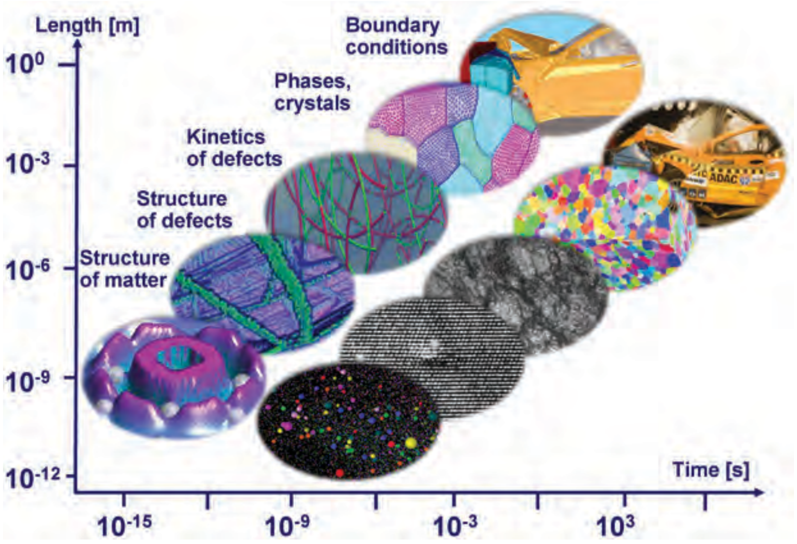


**Fig. 2:** *Scales in computational materials mechanics and how they match corresponding experiments. Here we show the specific example of crystal plasticity.*

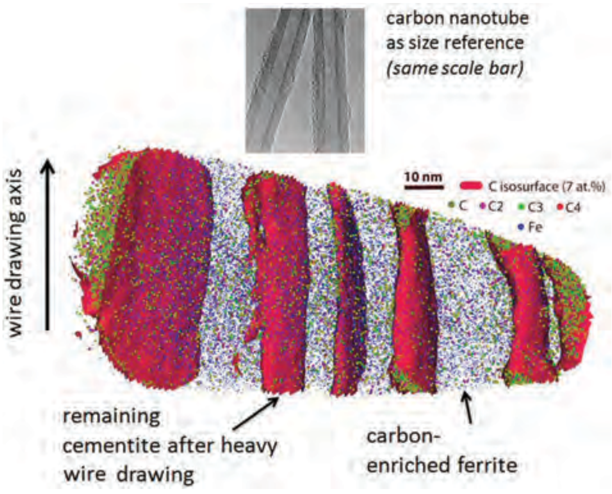


**Fig. 3:** *Heavily deformed pearlite is characterized by ferrite-cementite nanostructures with dimensions that are as fine as those of carbon nanotubes (Y.J. Li, S. Goto, R. Kirchheim) [41-43].*

of ductile, damage-tolerant maraging-TRIP steels by nanoscale precipitation of intermetallic phases and re-austenitization at interfaces [1,37,38].

Recent strategic scientific developments in the department were the opening of a new group on Atom Probe Tomography (APT) in 2010 [1,5,11,14]; the close collaboration with the department of J. Neugebauer on multiscale modeling of hardening and phase transformation phenomena as well as on computational thermodynamics [2-4,8]; and the strengthening of our metallurgical synthesis competence bundled in a new group on 'Combinatorial Metallurgy and Processing' that was opened in 2012 [39] (see p. 15).

The ability to probe the chemical and structural state of complex lattice defects (e.g. grain boundary segregation and nano-precipitates in Mn-steels [1] and pearlite [17,41-43] (see p. 107) by high resolution experiments (APT, TEM) does not only enable the direct comparison between experiments and atomistic simulations but it also opens a new pathway towards the atomic-scale characterization of lattice defects in functional materials. Examples are the chemical characterization of quantum-wells in LEDs [10], of decorated grain boundaries in CIGS and Si solar cells [11], and of nano-particles in soft magnetic alloys. In all these materials near-atomic characterization of defects is essential for understanding functional structure-property relations.

Projects demonstrating the strong inter-departmental links in the field of multiscale modelling are the *ab initio* prediction of phase stability and interface energies in complex steels (see p. 101), the *ab initio* guided development of ductile Mg alloys (p. 111), and Ti-based instable BCC and related Gum alloys which are characterized by large plastic yet hardening-free deformations (p. 113).

A further important step was the start of a new research group in 2012 on combinatorial metallurgy and processing (H. Springer) (see p. 15) [39]. This group conducts interdisciplinary research on alloy design and joining [40] of complex structural materials. We pursue a variety of new metallurgical synthesis methods, such as strip casting, amorphous steel solidification and specifically a new combinatorial high throughput approach that is specifically suited to systematically explore wide composition and property regimes of novel bulk structural alloys ('steel plant in a box') [39]. For this purpose we render the well-established combinatorial thin-layer approach into larger bulk quantities (kg-scale) and include – besides the variation in composition – also solidification, thermomechanical treatment, forming, and welding parameters. The aim is to probe large phase spaces of complex alloys under consideration of the required process parameters.

Close cooperation of the department exists with the institute's external scientific member R. Kirchheim on the fundamentals of the strength of heavily deformed Fe−C systems (see p. 107). This collaboration aims at a better understanding of the origin of deformation-induced alloying and the associated stabilization of sub-grain nanostructures via defectant effects, Fig. 3 [17,41-43]. Similarly, we closely cooperate with the Max-Planck Fellow G. Eggeler on elementary dislocation creep processes in high temperature alloys, Fig. 4.

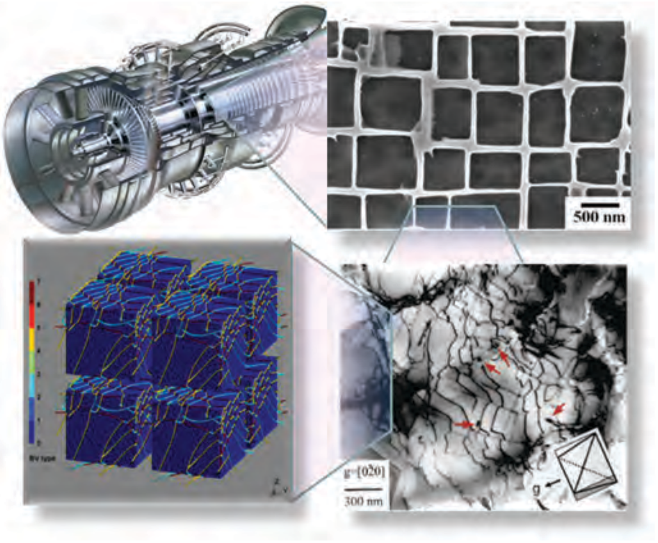


**Fig. 4:** *Scale-bridging analysis of the structure of Ni-base superalloys. Elementary dislocation kinetics and reaction rates during primary, secondary, and tertiary creep can be simulated using discrete dislocation dynamics (DDD) (B. Liu, A. Kostka, G. Eggeler).*

# Scientific Groups

## Introduction

The department has five permanent scientific groups,

- Theory and Simulation (F. Roters)
- Diffraction and Microscopy (S. Zaefferer)
- Alloy Design and Thermomechanical Processing (D. Ponge)
- Biological Materials (H. Fabritius)
- Combinatorial Metallurgy and Processing (H. Springer)

and five additional non-permanent scientific groups financed by third-party funds,

- Atom Probe Tomography (P. Choi, funded by Leibniz award)
- Adaptive Structural Materials (C. Tasan and B Grabowski, funded by ERC advanced grant)
- Computational Mechanics of Polycrystals (P. Eisenlohr, funded by MPG-FhG program of Max-Planck-Society)
- Theory and Simulation of Complex Fluids (F. Varnik, funded by MMM-initiative of Max-Planck-Society)
- Intermetallic Materials (F. Stein, M. Palm; group will be merged into new department of G. Dehm)

Owing to their extramural funding the latter initiatives are temporary groups. The project of P. Eisenlohr on the Computational Mechanics of Polycrystals was jointly funded after two subsequent evaluation workshops (2005, 2008) by the Max-Planck-Society and the Fraunhofer-Society for 3+3 years, 2005-2011. The group of F. Varnik on the Theory and Simulation of Complex Fluids was funded by the Max-Planck-Multiscale Modeling Initiative for 4 years, 2005-2009. Now it is carried further jointly through third party funds of MPIE and institutional funds of ICAMS (Interdisciplinary Centre for Advanced Materials Simulation) at Ruhr-University Bochum, Germany. The Atom Probe Tomography group, headed by P. Choi, has been established in 2010. It is financed through Prof. Raabe's Leibniz Award (German Research Foundation, DFG). The group for Adaptive Structural Materials, headed jointly by C. Tasan and B. Grabowski, is funded by an ERC advanced grant that was awarded in 2012 to D. Raabe and J. Neugebauer. The group for Intermetallic Materials was originally part of the department of the late Prof. Frommeyer and is currently cooperating with us on high temperature materials, iron-aluminides, and Laves phases. Since October 2012 it belongs to the new department of G. Dehm.

## Research Focus of Permanent Groups

### Theory and Simulation (F. Roters)

**Group Mission.** The group develops mechanism-based **crystal plasticity** constitutive models that describe the relationship between microstructures and mechanical properties of crystalline materials [16]. The approaches are based on mean-field formulations that describe the evolution of lattice defect structure such as dislocations and twins under given mechanical or thermal loading boundary conditions. The predicted defect densities enter into kinetic structure-property relations that translate them into strength and deformation measures [44,45]. Owing to the crystalline anisotropy of metallic alloys the constitutive laws assume a tensorial form both in their elastic and plastic formulations, i.e. they predict the defect evolutions on all crystallographic shear and twinning systems under external loads and their internal interactions. The formulations are built on dislocation densities (different types depending on the exact model), and can include mechanical twinning as additional deformation carrier. Interactions among dislocations and of dislocations with twins and grain boundaries can be considered. The resulting sets of nonlinear internal-variable differential equations are solved using either the **Finite Element Method** (CPFEM) [16,19,25,26,29,32-34,47,48] or a **Spectral Method** (CPFFT) [49,50], Fig. 5.

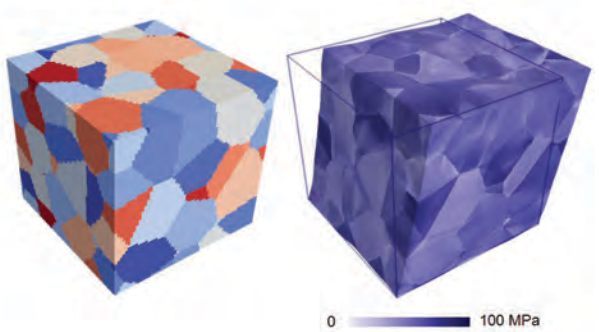


**Fig. 5:** *Simulation of simple shear using the spectral solver; left: volume element with periodic boundaries containing 50 grains with random orientation; 256x256x256 grid points; right: yz-component of first Piola-Kirchhoff stress after 20 % yz-shear deformation (F. Roters, M. Diehl, P. Eisenlohr, R. Lebensohn).*

**Research Highlights 2010-2012 including main trends over the past 6 years.** The most important highlight during the past years was the further development of a Spectral Crystal Plasticity (Fast Fourier) Method (**CPFFT**) together with R. Lebensohn from Los Alamos who spent a year in the group as Alexander von Humboldt Awardee [49,50]. This method was modified to enable the use of advanced non-linear constitutive models, such as described above, and equipped with a robust integration algorithm. Furthermore, a regrinding capability has been developed to ensure that the gradual micromechanical distortions do not impede convergence. The fundamental advantage of this approach is that FFTs can solve the underlying constitutive elasto-plastic equations under periodic boundary conditions about orders of magnitude faster than FEM solvers at much lower memory costs. Also CPFFT has the advantage that it can directly be applied to EBSD or other fixed-grid microstructure data sets circumventing the requirement to reconstruct complicated mesh geometries as it should be done for corresponding CPFEM simulations. The novel method is mature and currently successfully applied to full-field simulations of deformation heterogeneity in dual phase steels, porous alloys, and ice mechanics.

Another field of activity was the application of advanced CPFEM simulations to the prediction and better understanding of shear banding in crystalline materials [16]. Shear bands are the most frequently observed yet least understood mesoscopic, collective plasticity mechanism. They play an essential role in strain hardening, strain localization, texture evolution, and damage initiation. We found that shear banding is strongly orientation dependent. For example Copper and Brass-R-oriented crystals (FCC lattice) show the largest tendency to form shear bands and build up an inhomogeneous texture inside the shear bands. Shear banding in these crystals can be understood in terms of a mesoscopic softening mechanism. The predicted local textures and the shear banding patterns agree well with experimental observations in low SFE FCC crystals [47,48].

The progress in these various fields of polycrystal mechanical modeling achieved by our group in terms of methods development and applications was recently published as an overview article in Acta Materialia [16] and is since its appearance the most downloaded publication of all papers published in this journal. The software developed during the last years was released to the public domain as Düsseldorf Advanced MAterials Simulation Kit (DAMASK) and can be downloaded from the internet: http://damask.mpie.de. It is already used by several research groups in Europe and the US.

Another growing field of interest are **discrete dislocation dynamics** (DDD) simulations [35,36]. These models are built on three assumptions. First, the distortions around lattice dislocations are treated as linear elastic fields and are solved piecewise (i.e. for a portion of the dislocation) via the Volterra equation and Hooke's law. Second, all dislocation lines are decomposed into sequences of connected segments. Third, the dynamics of each segment is solved using a damped viscous form of the equation of motion considering long and short range elastic interactions among all dislocation segments via the Peach-Koehler equation plus external loads. The simulations using the massively parallel ParaDiS code of the Lawrence Livermore National Laboratory (USA) [51] are computationally highly demanding so that they run on the Blue Gene/P high performance computer of FZ Jülich on up to several thousand processors.

In this field we also aim twofold: First we improve the theoretical foundations of the approach further (e.g. by including dislocation climb) and second apply it to problems where the simulation of small sets of interacting dislocations provides insights into the underlying micromechanics.

Main projects pursued by discrete dislocation simulations are the strengthening effects of small angle grain boundaries [35,36], creep in Ni-based superalloys (Fig. 4), and dislocation patterning.

### Microscopy and Diffraction (S. Zaefferer)

**Group Mission.** The group pursues two main missions. The first one is the development of advanced microstructure characterization methods focussing during the past years on SEM- and FIB-SEM based approaches. Specific focus is placed on diffraction methods such as high angular and spatial resolution orientation microscopy (**HR EBSD**) in the SEM, **electron channelling contrast imaging** (ECCI), **internal stress** determination via SEM/EBSD, and 3D electron backscatter diffraction (**3D EBSD**, tomographic EBSD) [6,15,18-22,55-57].

The second main objective of the group lies in the application of these advanced characterization methods with the aim to understand and quantify with high crystallographic precision microstructure evolution phenomena associated with transformation and plasticity mechanisms and the proper characterization of the dislocations and interfaces involved. The metallurgical phenomena of interest are mainly in the fields of polycrystal crystal plasticity (mainly steels, Ni-alloys, and Mg-alloys), twinning and martensitic transformation (in steels with twinning or transformation induced plasticity (TWIP or TRIP)) as well as annealing phenomena.

The group operates several instruments. Among these is a Zeiss Crossbeam XB1560 FIB-SEM for 3D EBSD investigations, a JEOL JSM 6500 F SEM (both with field emission gun), and a Camscan 4 tungsten filament SEM. These instruments are equipped with EBSD analysis hardware and allow mounting micro-deformation machines for *in situ* deformation testing. A heating stage is also available for conducting *in situ* transformation experiments. For ECCI a eucentric 5-axis goniometer stage has been custom-designed by Kleindiek nanotechnology. Transmission electron microscopy (TEM) is performed on a Phillips CM 20. This instrument is equipped with a large angle, high dynamics camera (Olympus) for image and diffraction pattern acquisition and the software TOCA for on-line crystallographic analysis. Furthermore, several XRD goniometers are available.

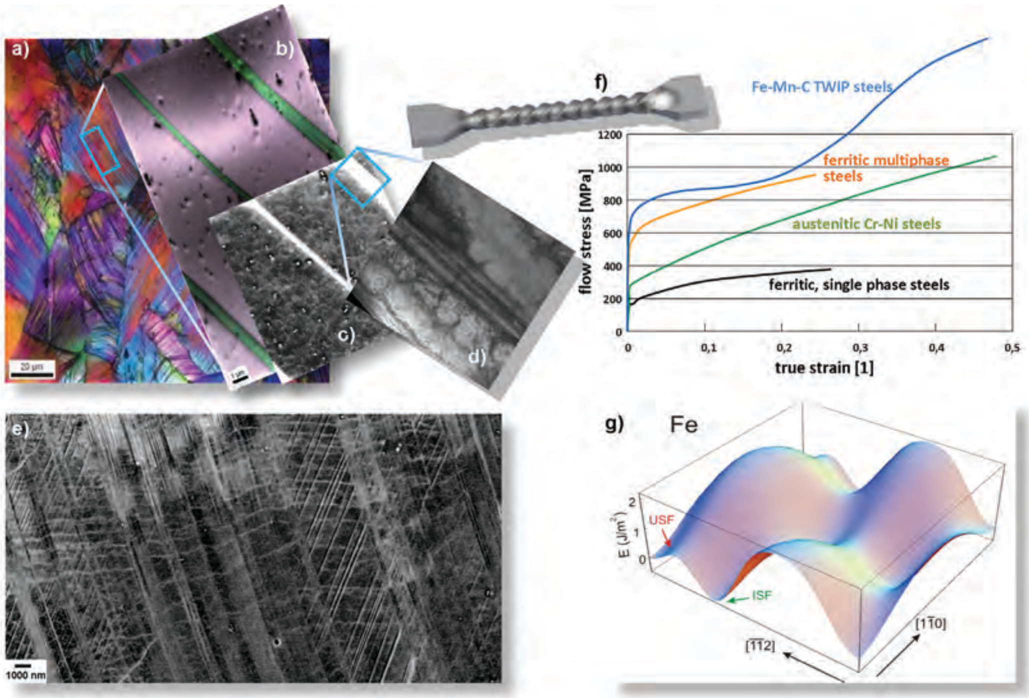


**Fig. 6:** *Example of a Fe-Mn TWIP steel (22 wt.% Mn, 0.6 wt.% C) where an instability analysis (in terms of the stacking fault energy) is used to design the desired transformation behaviour (here: evolution of twins during deformation). The result is a strong increase in both, strength and ductility. Slight changes in the chemical composition modify the stability of the FCC Fe-Mn-C matrix against mechanical twinning and can shift the system towards preferring other transformations (e.g. ε-martensite, tetragonal martensite). The images on the left and side reveal the hierarchical microstructure after an equivalent strain of about 20% which can – irrespective of its enormous complexity – be understood in terms of the stacking fault energy. The images on the left hand side are obtained via a) EBSD (electron back scatter diffraction) image; b) high resolution EBSD; c) ECCI (electron channelling contrast imaging) revealing also dislocations (see also wide-field of view ECCI micrograph (e) at the bottom); and d) TEM (transmission electron microscopy). The right hand side shows the enormous increase in the strength-ductility profile of this novel alloy compared to conventional materials that are plotted in the same diagram. The results of the ab initio prediction of the generalized γ-surface (by department of J. Neugebauer) is shown in g) and allows to extract critical information such as the intrinsic stacking fault (ISF) energy or its kinetic barrier to create it (unstable stacking fault – USF) energy (I. Gutierrez-Urrutia, J. Neugebauer).*

**Research Highlights 2010-2012 including main trends over the past 6 years.** Highlight activities of the group during the past two years were the development of a new approach to electron channelling contrast imaging (ECCI), named “controlled ECCI”, or cECCI [15,21,22], Fig. 6. This method improves the existing ECCI method in a way that it uses EBSD to determine the crystal orientation. Based on this the optimum sample alignment for obtaining good channelling contrast is calculated using the computer software TOCA [52]. A dedicated eucentric goniometer stage is then used to move the sample into the calculated position for imaging of dislocations and other crystal defects in the SEM. The approach offers excellent opportunities for the efficient quantification of substructure features at a large field of view that were not accessible so far to SEM characterization, Fig. 7. It can be combined with EBSD maps so that we are now

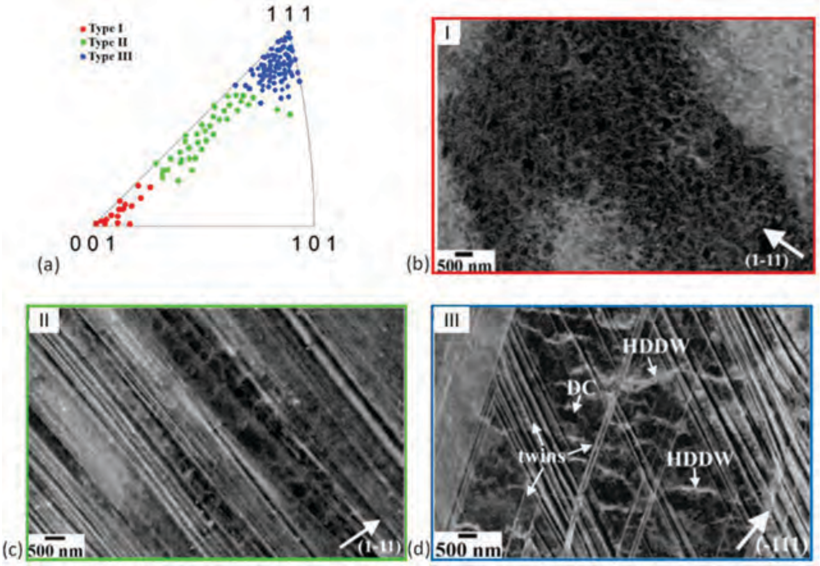


**Fig. 7:** *Different deformation structures observed with controlled electron channeling contrast imaging (cECCI) in a TWIP steel deformed in a tensile test to a true strain of 0.3. (a) Standard orientation triangle indicating the tensile direction in crystal coordinates for different crystals in the material. Crystals with different characteristic deformation structures are classified as type I, II and III. (b) Dislocation cell structure typical for grains of type I. (c) Dense single system twin lamellae, typical for grains of type II. (d) Several twin systems, typical for grains of type III (from [21]). DC: dislocation cell, HDDW: highly dense dislocation walls.*

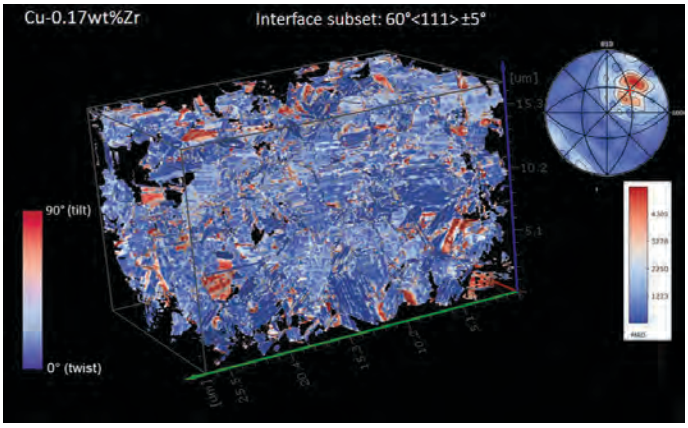


**Fig. 8:** *Characterization of the tile and twist fractions of the 60° <111> grain boundary family in a deformed Cu-Zr sample by 3D EBSD (P.J. Konijnenberg).*

capable of conducting detailed microstructure quantification mappings of orientations together with its inherent dislocation substructure in the same experiment. Tedious and time consuming TEM investigations of dislocation structures that provide a small field of view thus may become obsolete in a number of cases.

A second focus of the group lies in the improved analysis of 3D EBSD data with respect to the characterisation of interface segments. As was shown in the last bi-annual reports it is in principle straight forward to extend the 2D EBSD (electron backscatter diffraction)-based orientation microscopy technique to a 3D technique by collecting sequential sets of 2D maps by serial sectioning, e.g. by mechanical or chemical polishing or sputtering with a focussed ion beam (FIB). 3D EBSD offers unique and novel features to characterize microstructures, in particular the full, 5-parameter grain boundary description but also, for example, the description of connectivity of phases, 3D morphology of crystals, or the determination of geometrically necessary dislocation (GND) densities [20,33]. The 3D EBSD data can be analysed in two approaches, either as volume pixels (voxels) or by rendering interfaces and boundaries. While the former method has been discussed in the past reports the interface segment reconstruction is currently the most important pending problem. In our current approach the grain boundary reconstruction consists of two sequential steps; namely, first, in identifying the boundary surface and subsequently translating this surface into a mesh of triangles. A well-known method for boundary reconstruction is the Marching Cubes (MC) algorithm which has been applied for boundary reconstruction from orientation voxels before. The standard MC algorithm suffers from several inherent ambiguities. These ambiguities can be solved by disassembling each cube into unambiguous tetrahedra, resulting in the so-called Marching Tetrahedra (MT) algorithm which leads to better results. Once grain boundaries are established as sets of triangles these boundaries have to be smoothed before any quantitative statements about spatial or crystallographic features of the boundaries can be made. Different smoothing algorithms have been developed and tested. Furthermore a number of algorithms have been developed to display and interpret the crystallographic nature of boundaries in the 5 parameter grain boundary space (3 parameters describing the misorientation and 2 the boundary normal) [53], Fig. 8.

The algorithms used for interface characterization are part of a large software suite, Qube, which has been developed over the last two years mainly by P. Konijnenberg. It embeds under a user-friendly software interface powerful tools for 3D microstructure characterization. This includes, for example, the calculation of GND densities from the 3D orientation field curvature, the calculation of 3D orientation gradients, 3D rendering of interfaces and the quantitative calculation of grain and boundary textures (see p. 117).

A further recent focus of the group is placed on the development and use of EBSD-based methods for the measurement of local elastic (lattice) and plastic strain. In one approach, followed by T. Jaepel, a cross-correlation technique is used to measure the distribution of lattice strains inside of individual crystals of a polycrystal or in single crystal samples. The fact that this technique requires reference patterns of similar orientation limits this technique to special cases and does not allow determining absolute levels of internal stresses. A second approach, therefore, uses a reference pattern-free algorithm to measure absolute lattice strains. A third approach, finally, is followed by F. Ram, who developed the Kikuchi bandlet method to determine with highest accuracy the position of Kikuchi cones from EBSD patterns. These data can then be used to determine the geometrical pattern origin and the lattice distortion with high accuracy. The Kikuchi bandlet method can also be used to determine, from the Kikuchi band profile, the crystal defect density (i.e. the total dislocation density) in the electron beam interaction volume.

Related to the measurements of stress and strain are research initiatives which use *in situ* deformation tests to observe strain hardening mechanisms in various materials. Besides local strain measurements with the above mentioned techniques these projects use ECCI and digital image correlation to quantify the local plastic strain. The project is pursued by C. Tasan.

Finally, several research initiatives deal with the statistical representativeness of local property measurements. In a project on low alloyed TRIP steels the statistical representativeness of EBSD for phase and texture determination was studied and a new software tool for large area measurements

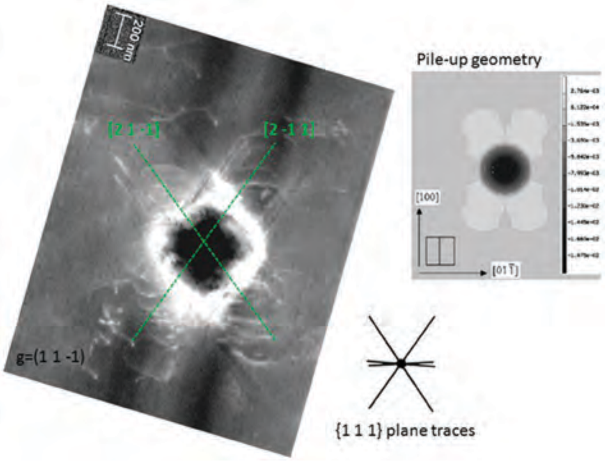


**Fig. 9:** *Dislocation structure around a nanoindent into an undeformed TWIP steel surface observed by cECCI. Dislocations are emitted out of the nanoindent in <112> directions. This corresponds to the expected pile-up symmetry displayed on the right side calculated by crystal plasticity FEM (J. Zhang).*

developed [54]. Another project, pursued so far by J. Zhang, deals with the analysis of nanoindentation for measurement of residual stresses. The results are interpreted in terms of dislocation structures that are observed using the cECCI technique, Fig. 9.

### Alloy Design and Thermomechanical Processing (D. Ponge)

**Group Mission.** In the past 6 years the group worked mainly on microstructure design and optimization of the mechanical properties of carbon-manganese steels via grain refinement by thermomechanical treatment [55,58-63]. Main examples were the design of advanced ultrastrong spring steels and bulk ultra-fine grain steels. More specific the main alloy systems addressed were ultra fine grained plain C−Mn steels and dual phase (DP) steels for light-weight automotive applications [55, 58-63]. The microstructure-oriented optimization of microstructures and properties of novel complex engineering steels via thermomechanical treatment requires a detailed understanding of the relations between processing and microstructure evolution on the one hand and the relations between microstructures and mechanical properties on the other. This two-fold strategy is essential in this field as no direct link exists between processing and properties.

In addition to the development of optimal thermomechanical processes, in the past few years projects increasingly included mechanism-based alloy design strategies [1,15,21,22,64,65]. The reason is that alloy development is an ideal addition to thermomechanical processing as it gives access to a larger variety of bulk phase transformations, precipitate strategies, and grain refinement mechanisms. The joint design of both, novel alloy variants in accord with thermodynamic and kinetic prediction tools and adequate thermomechanical processing hence describes the current research strategy of the group (see p. 101). In order to probe the composition phase space more efficiently the team closely interacts with the new group on combinatorial metallurgy and processing (see p. 15).

**Research Highlights 2010-2012 including main trends over the past 6 years.** During the past two years the group was mainly concerned with the development of a new alloy class, namely, Mn-based lean maraging-TRIP steels [1,37,38]. The concept is based on combining the TRIP effect with the maraging effect (TRIP: transformation-induced plasticity; maraging: martensite aging) (see p. 101). The Fe-Mn-based maraging-TRIP alloys combine different hardening mechanisms. The first one is the formation of strain-induced martensite (alloys with 0.01 wt.% C and 12 wt.% Mn have retained austenite fractions up to 15 vol.%) and exploits the same hardening principles as TRIP steels. The second effect is the strain hardening of the already transformed ductile, low carbon α'- and ε-martensite phases and of the remaining retained austenite. The third effect is the formation of nano-sized intermetallic precipitates in the martensite during heat treatment. These precipitates have high dispersion owing to the good nucleation conditions in the heavily strained martensite matrix in which they form. The fourth one is the formation of nanoscaled re-austenitization layers on the formerly segregation-decorated martensite grain boundaries during the maraging heat treatment. This combination of mechanisms leads to the surprising property that both strength and total elongation jointly increase upon martensite aging (e.g. 450°C, 48 hours) reaching an ultimate tensile strength of nearly 1.3 GPa at an elongation above 20% [37,38].

Specifically the occurrence of nano-scaled re-austenitization layers at the martensite grain boundaries seems to have a beneficial effect on the blunting of cracks rendering the martensite ductile. This effect could be realized in a second alloy class, namely, in a martensitic Fe–13.6 Cr–0.44 C (wt.%) martensite steel. After tempering the martensite was rendered into an ultra-high-strength ferritic stainless steel with excellent ductility. The nanoscale austenite reversion mechanism that occurred in this alloy is coupled to the kinetic freezing of carbon during low-temperature partitioning at the interfaces between martensite and retained austenite and to carbon segregation at martensite–martensite grain boundaries. An advantage of austenite reversion is its scalability, i.e. changing tempering time and temperature tailors the desired strength–ductility profiles. E.g. tempering at 400 °C for 1 min produces a 2 GPa ultimate tensile strength (UTS) and 14% elongation while 30 min at 400 °C results in a UTS of 1.75 GPa with an elongation of 23% [14].

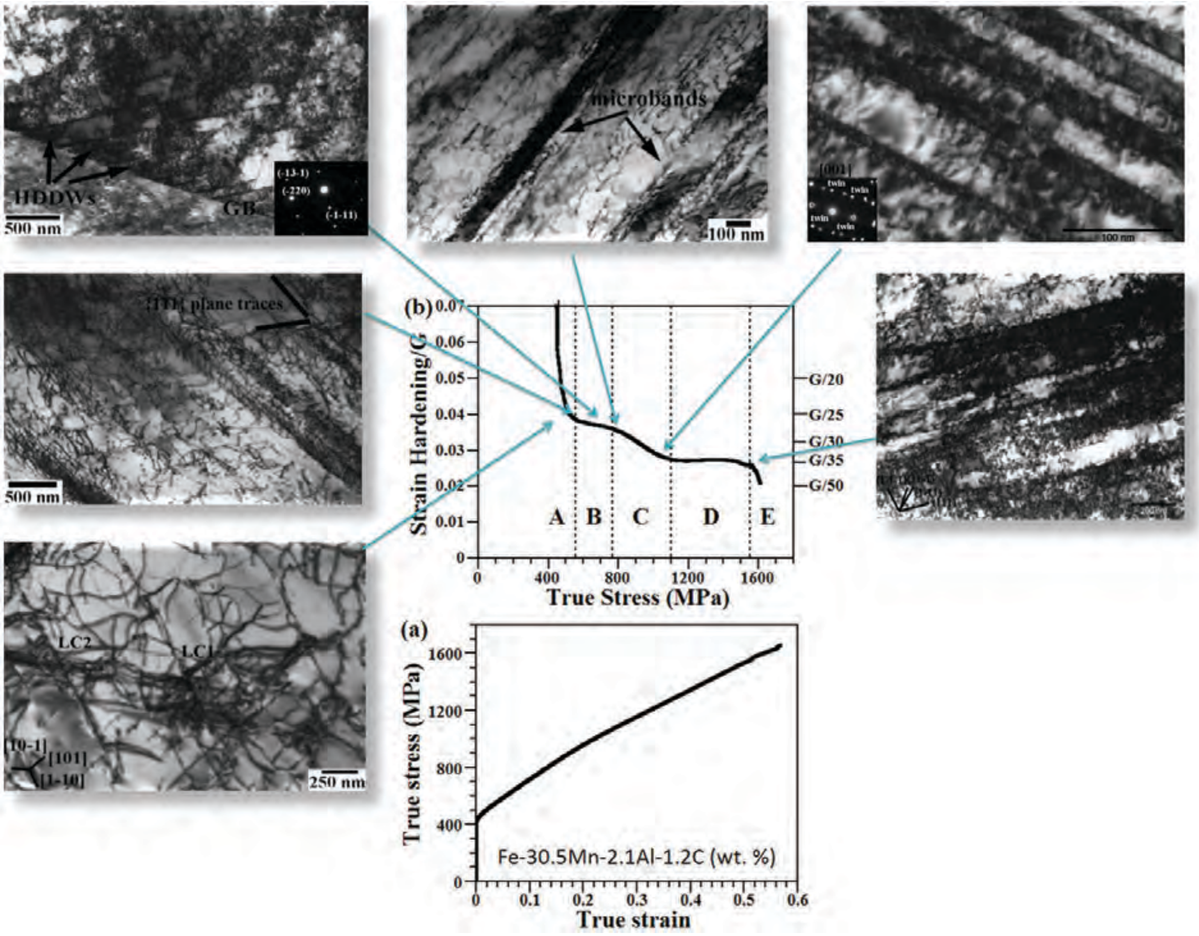


**Fig. 10:** *Non-heat treated Fe–30.5Mn–2.1Al–1.2C (wt.%) weight-reduced steel with fcc crystal structure. Characterization of the different strain hardening stages using TEM analysis (I. Gutierrez-Urrutia) [15].*

A third group of steels that is being addressed jointly by this group and the new group on combinatorial alloy design are weight-reduced austenitic or austenitic-ferritic steels. These are steels with up to 30 wt.% Mn, up to 8 wt.% Al and up to 1.2 wt.% C which are sometimes also referred to as TRIPLEX steels owing to their two- or three phase composition. They are characterized by about 10% reduced specific weight and excellent stress-ductility profiles, Fig. 10. Depending on heat treatment and composition they can contain nanostructured kappa carbides [39].

### Biological Materials (H. Fabritius)

**Group Mission.** Most biological materials with structural functions consist of an organic matrix of structural biopolymers like collagen and chitin, which is modified and reinforced with different proteins and in many cases also with biominerals. The most prominent examples like the bones of vertebrates, the exoskeletons of arthropods, and mollusk shells are known to possess optimized function-related physical properties (e.g., mechanical properties: stiffness-to-density ratio and fracture toughness). The origins of these properties, particularly the underlying structure/composition/property relations, are the research subject of this group [66-70].

In our work on mineralized chitin-based arthropod cuticle we found out that the specific design and properties at the nanoscale contribute significantly to their macroscopic properties. Evidently, the overall properties depend on the specific microstructure at all levels of hierarchy [8,71]. However, especially the properties at small length scales are experimentally hard, if not impossible, to access due to methodological constraints. Hence, multiscale modeling that can systematically describe and investigate materials properties from the atomistic scale up to the macroscopic level has become a major approach in the group in close cooperation with the department of J. Neugebauer to tackle the structure/property relations of biological organic/inorganic nanocomposites. The method has been applied to bone and crustacean cuticle [8,72,73]. In addition to modeling fully differentiated structural composites, the approach has also been applied to model the mechanical properties of individual constituents and explain the structure/property relations on increasingly complex structural hierarchy levels.

**Research Highlights 2010-2012 including main trends over the past 6 years.** The cuticle of *Arthropoda* is a continuous tissue that covers the entire body. In order to function as an exoskeleton, it has to form skeletal elements with physical properties that are adapted to specific functions which are very diverse, like providing mechanical stability in the shell of body segments, elasticity in arthrodial membranes, or wear resistance and friction reduction in joint structures and mandibles. The required properties for each skeletal element are adjusted by local modifications in structure and composition. The transitions between parts with different properties are brought about by structural interfaces, which are generated on different hierarchical levels. Employing our established experimental approaches, we investigate the nature of such interfaces in functionally differentiated cuticle parts such as mandibles of *Crustacea* species with different feeding habits and transitions between mineralized load-bearing cuticle and unmineralized arthrodial membranes. Since our theoretical multi-scale model can only predict the average elastic properties of cuticle, we developed a hierarchical model for the elasto-viscoplastic cuticle properties at large deformations using a Fast Fourier Transforms (FFT) approach that is able to describe the local development of stress and strain fields within the material, including those at the interfaces.

In addition to serving as exoskeleton, the cuticle of *Arthropoda* also plays an important role for the ecophysiology of the organisms by forming photonic crystals that generate colors through scattering of light by photonic band gap materials. We use the cuticle of various beetle species to both experimentally and theoretically investigate the structure and resulting optical properties of photonic crystals as found in the small scales covering the beetle *Entimus imperialis*. They consist of a diamond-structured cuticular network and air, where the structural parameters are optimized to produce the brightest colors possible by maximizing band gaps width. In some scales, this effect is turned into the opposite, transparency, through alteration of the refractive index contrast by substitution of the air with $SiO_2$. In collaboration with the group of Prof. Zollfrank (TU Munich), this biological photonic crystal has been biomimetically transferred into identical silica replicas with tunable structural parameters. Based on these results, we started to combine experiments and theory to develop biomimetic photonic crystals with tailored optical and mechanical properties for potential mechanochromic applications (see p. 139).

Over the last years, we expanded our studies on structure/property relations in biological composites beyond mechanical properties with particular focus on multifunctional parts, property transitions and different and/or unusual property combinations with the aim to expand the knowledge necessary to develop corresponding synthetic materials.

### Combinatorial Metallurgy and Processing (H. Springer)

See separate presentation of this new initiative on page 15.

## Overview on Non-Permanent Groups and Their Research Focus in the Past Years

### Atom Probe Tomography (P. Choi, funded by Leibniz award)

**Group Mission.** The group was opened in 2010 and has since then seen very rapid growth in terms of topics and personnel. Atom Probe Tomography (APT) is a characterization technique enabling spatially resolved chemical analyses of materials at sub-nanometer resolution (in-plane: ≈0.2 nm; in-depth: ≈0.1 nm) [1,9,11,14,17,41-43]. The instrument (Imago Scientific Instruments, LEAP 3000X HR) is equipped with a local electrode, a wide-angle reflectron, a high-speed delay line detector system as well as an ultrafast laser with a pulse width of 10 ps and wavelength of 510 nm. Such an instrument design has numerous advantages over conventional atom probes, particularly regarding the analysis of alloys with complex chemical composition. The local electrode enhances the electric field at the specimen and allows fast pulsing (max. 200 kHz) at low voltage. A high-speed delay line detector system provides fast data acquisition rates of up to 2 Mio ions/min. Due to the proximity between specimen and detector, the field of view can be as large as 200 nm. As a result, large volumes, which can contain up to several hundred millions of atoms, can be probed within a few hours. The wide-angle reflectron substantially enhances the mass resolution of this instrument. Complex multi-component systems can therefore be analyzed at high compositional accuracy. Furthermore, impurity concentrations as low as few tens of ppm can be detected. The ultrafast laser extends the applicability of this technique to materials having low electrical conductivity such as semiconductors and ceramics [10,11].

The research objectives of the group are in two fields. The first one is the near-atomic scale analysis of interface-related phenomena, such as segregation, partitioning and associated local thermodynamic and kinetic phenomena, for instance phase transformations at grain boundaries [1,14]. Owing to the capability of instrument to probe samples with small electrical conductive in Laser excitation mode, increasingly also interfaces and quantum well structures of functional polycrystalline materials are studied.

The second aim of the group lies in comparing atom probe tomography observations quantitatively with theoretical predictions. For this purpose we use ThermoCalc and Dictra approaches as well as *ab initio* predictions in conjunction with kinetic Monte Carlo methods. While the former set of statistical simulations are mainly conducted in close collaboration with G. Inden and the group of D. Ponge

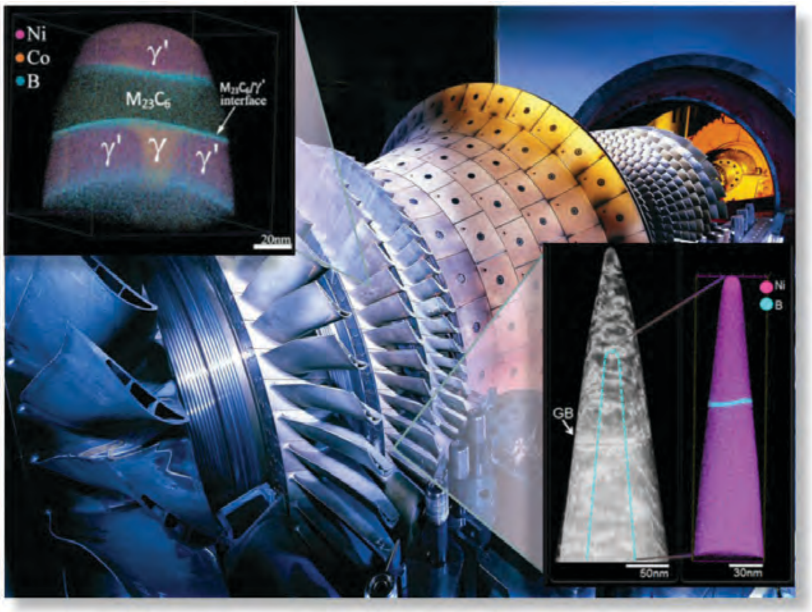
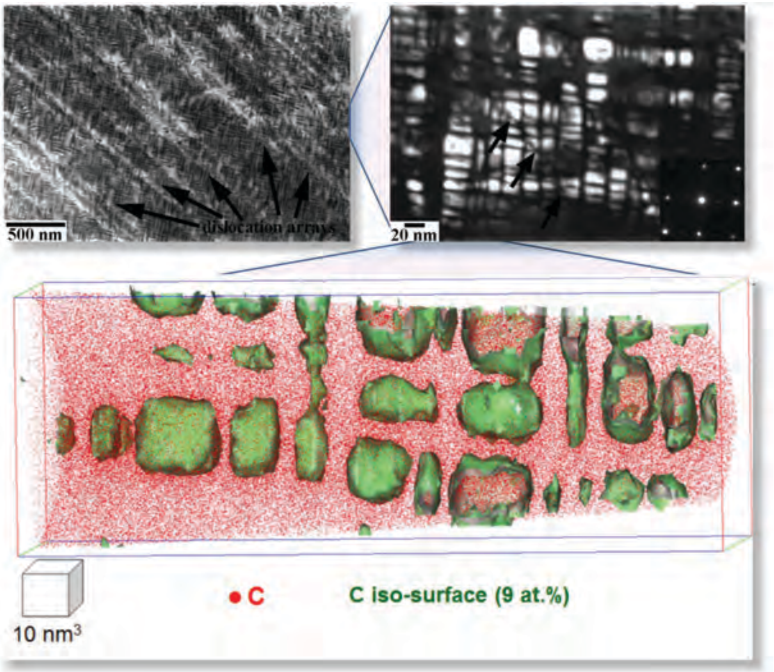


**Fig. 11:** *Use of atom probe tomography for the analysis of the atomistic details of carbide formation and boron-decoration of interfaces in Ni-base alloys that are developed as blade components for power plant turbines (D. Tytko, I. Povstugar) [5].*

**Fig. 12:** *Formation of nano-sized kappa-carbides in weight-reduced Fe−Mn−Al−C steel using ECCI, TEM, and APT (J. Seol, P.-P. Choi, I. Gutierrez-Urrutia).*



(Alloy Design and Thermomechanical Processing) the latter calculations are done in the department of J. Neugebauer in the group of T. Hickel (Computational Phase Studies).

**Research Highlights 2010-2012 including main trends over the past 3 years.** The group studies both, functional and structural materials. Examples are thin-film solar cells (based on Cu(In,Ga)Se$_2$ and CdTe) and light-emitting diodes (based on III-V semiconductors) [10], as well as Al- and Cr-Nitride multilayer hardcoatings. Regarding metallic alloys essential research topics are the formation of nanoscaled re-austenitization films on martensite grain boundaries in Fe−Cr−C and Fe−Mn steels; interfaces in Ni-based superalloys, Fig. 11 [5]; the stabilization of ferrite nanograins in mechanically alloyed and heavily deformed pearlite by massive carbon decoration of the grain boundaries [41-43]; the formation of Cu-based nano-precipitates in Fe−Si−Cu soft magnetic steels; partially crystalline soft magnetic metallic glasses; and nano-structured carbides in weight reduced Fe−Mn−Al−C steels, Fig. 12. The group is currently financed through the funds of Prof. Raabe's Leibniz Award (German Research Foundation, DFG).

### Adaptive Structural Materials (C. Tasan and B. Grabowski, funded by ERC advanced grant)

See separate presentation of this new initiative on page 13.

### Max-Planck-Fraunhofer Group on Computational Mechanics of Polycrystals (P. Eisenlohr)

**Group Mission.** The group was founded in 2005 as the first joint research group between the Max-Planck-Society and the Fraunhofer-Society (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg). Funding was jointly provided by the Max-Planck and Fraunhofer-Societies. The group develops theoretical approaches for the mechanics and damage initiation of textured polycrystalline matter with the aim to promote its use for industrial applications such as encountered in the fields of metal forming and microstructure mechanics.

**Research Highlights 2010-2012 including main trends over the past 6 years.** In the past years the group has pursued the following goals in collaboration with the group for Theory and Simulation (F. Roters) [16,50,74,75]: The first direction was the development of an advanced homogenization schemes [77,78]. This model calculates the stress for a group of interacting crystals under an external given boundary condition considering internal relaxations among the abutting crystals. Such approaches allow polycrystal simulations at a scale above the full-field crystal plasticity finite element schemes. A novel approach, referred to as Relaxed Grain Cluster model (RGC), was developed and successfully applied to steels. This method does not only improve existing homogenization schemes for polycrystal mechanics but it can also be used as a homogenization method for multiphase polycrystalline materials, such as for instance for TRIP steels.

The second aim of the group was the development of advanced constitutive models that describe the individual deformation behaviour inside the crystals. Of particular interest was the development of constitutive models that include deformation twinning and its interaction with dislocation slip [44]. Also, an improved mean-field dislocation flux model is being developed that communicates dislocation streams and balances reaction as well as annihilation rates among neighboring field integration points according to the local boundary conditions. This flux formulation accounts for geometrically necessary dislocations and the associated local stress peaks.

The third field is the role of heterogeneous deformation on damage nucleation at grain boundaries in single phase metals [26]. This work is done in close cooperation between our department (P. Eisenlohr) and T.R. Bieler and M.A. Crimp from Michigan State University in East Lansing, USA, and Professor D.E. Mason from Albion College in Albion, USA. The project aims to understand which mechanical criteria determine where and why cracks or voids form in a strained polycrystal particularly at grain boundaries. This project is jointly funded by the US and German research foundations, NSF and DFG.

### Theory and Simulation of Complex Fluids (F. Varnik)

**Group Mission.** The group for the simulation of complex fluids is rooted both at the ICAMS at Ruhr-University Bochum and at MPIE. Its field is the study of the structural and mechanical properties of complex multiphase and colloidal fluids [79-85]. Typically, fluids can be deformed already when being exposed to weak forces such as in the case of shear melting. This effect often goes along with a drop in shear viscosity upon increasing shear rate. This phenomenon is referred to as shear thinning. The relation between the stress and deformation for a complex fluid is often non-linear. There is a wide field of applications of complex fluid mechanics, for instance in polymer processing, metallurgical processing [86,87], and biology [81,82]. As a modeling method we mainly use the lattice Boltzmann method (LBM) and multiphase variants thereof [62-68]. LBM is well suited for the numerical calculation of fluid flow, heat, and solute transport. Unlike Navier-Stokes solvers, the LBM mimics flows as collections of pseudo-particles that are represented by a velocity distribution function. These fluid portions reside and interact on the nodes of a grid. System dynamics emerge by the repeated application of local rules for the motion, collision, and re-distribution of the fluid particles. The method is an ideal approach for mesoscale and scale-bridging simulations owing to its computational efficiency and versatility in terms of constitutive description of its pseudo-particles. Also it can be efficiently cast into parallel codes. In particular, LBM exhibits good numerical stability for simulating complex fluids, such as multi-phase and multi-component flow phenomena under complicated boundary conditions. Since LBM describes fluid motion at the level of the distribution functions, it can be naturally coupled with related simulation techniques such as cellular automata or phase field models [86,87].

**Research Highlights 2010-2012 including main trends over the past 6 years.** The group investigates problems in micro-fluidics such as inhomogeneous diffusive broadening, droplet and contact dynamics on chemically and topographically patterned substrates as well as flow between topographically rough walls. On the nano-scale, on the other hand, the group focuses on the effects of thermal fluctuations on droplet dynamics. Furthermore, the group has also developed efficient parallel LBM variants that are recently particularly used for the study of blood flow mechanics [64,68]. These studies have proved very fruitful with a number of interesting observations as well as theoretical predictions, the latter being verified by independent computer simulations. To name just a few examples, we mention the observation of instantaneous droplet motion on a gradient of texture, and the discovery of new types of wetting states in the case of small droplets with a size comparable to the roughness scale [84].

### Intermetallic Materials (F. Stein, M. Palm)

The group for Intermetallic Materials was initially part of the department of the late Prof. Frommeyer and is currently closely cooperating with us on high temperature materials and iron-aluminides. Since October 2012 it is part of the new department of G. Dehm (see p. 91).

# Key Interdisciplinary Research Fields of the Department

The groups introduced above represent the main **competence centers** of the department. Our mission, however, aims beyond these fields, i.e. we additionally pursue a number of joint **grand challenges** tackling of which requires efficient bundling of these skills. Some cross-disciplinary and cross-departmental topics are described in the **research highlight** section. Here, we introduce some main inter-disciplinary research fields where the different groups team up and conduct long-term fundamental research. In the past years three main areas prevailed, namely:

I. Designing intrinsically nanostructured metallic alloys

II. Advanced characterization of complex materials

III. Predictive and quantitative multiscale models

In the following we give a concise introduction into our respective approaches:

## I. New materials: Mechanism-oriented design of intrinsically nanostructured metallic alloys

The design of advanced high strength and damage tolerant metallic alloys for energy, mobility, safety, health and infrastructure applications forms the engineering and manufacturing backbone of our modern society. Examples are creep-resistant steels and Ni-alloys [5] in power plants and plane turbines; ultrahigh strength steels [1,14,21,39,44], Ti-, and Mg-alloys for light-weight mobility and aerospace design [2,3]; metallic glasses for low-loss functional components; or biomedical Ti-implant alloys in aging societies [4].

Since the Bronze Age the design of novel metallic alloys was based on trial and error approaches, owing to the complexity of the physical and chemical mechanisms involved and the engineering boundary conditions imposed during synthesis and manufacturing. This traditional method has two shortcomings. First, current alloy design is not based on systematic design rules but on metallurgical experience alone. This renders the development of novel alloys inefficient. Second, the increase in strength via traditional hardening mechanisms such as solute solution, increase in dislocation density, or second phase precipitates, albeit leading to a high strength level, always causes a dramatic decrease in ductility, i.e., making the material brittle and much more susceptible for failure.

The joint research field of designing new metallic alloys aims at solving this inverse strength-ductility problem: The recent achievements in *ab initio* modeling and atomic scale characterization methods presented above and in some of the highlight papers open a fundamentally new pathway to the systematic and knowledge-based design of next generation metallic alloys. The objective is to use these methods to identify and utilize strengthening mechanisms that enable us to overcome the inverse relationship between strength and ductility. The key idea to better reconcile high strength and high ductility is to incorporate second phases into bulk alloys that are close or even beyond their mechanical and thermodynamic stability limit. While this sounds at a first glance counterintuitive – in the end we aim at materials with superior mechanical stability – the well-controlled inclusion of topologically confined phases with reduced stability provides a method to stimulate finely dispersed deformation-driven displacive transformations. Optimizing the degree of instability, dispersion, and volume mismatch associated with transformations allows one to tailor compliant microstructures that reduce damage initiation. The novelty of the approach is that the transformation occurs only in regions with high local stress concentrations and, hence, acts as spatially localized self-organized repair mechanisms against localization softening and premature internal damage owing to its associated strain hardening and compressive stresses. This new principle of designing higher mechanical stability of metallic alloys by including instable phases carries the potential to deviate from the inverse strength-ductility principle that currently sets a limit to advanced engineering alloys.

The cornerstones for this systematic alloy design approach are a better understanding of the thermodynamics and kinetics of instable phases; the bulk combinatorial lean synthesis, processing, and probing of corresponding alloy classes; and the discovery of the governing strain hardening mechanisms and their interactions.

Regarding the first aspect, the use of novel theoretical tools such as ***ab initio*** simulations (department of J. Neugebauer) together with established thermodynamic and kinetic simulation tools such as **ThermoCalc** and **Dictra**, and the conjunction with local experimental analysis are conducted to discover composition and processing niches where phase instability can be exploited to lead to stronger and yet more ductile mechanical response. The second method, namely the combinatorial manufacturing of corresponding bulk specimens is described on p. 15. The third aspect, i.e. the understanding of new strain hardening effects requires the use of careful high resolution and at the same time wide field of view characterization methods such as the quantitative electron channelling contrast imaging, TEM, and atom probe tomography. Regarding the interplay of the thermodynamics of

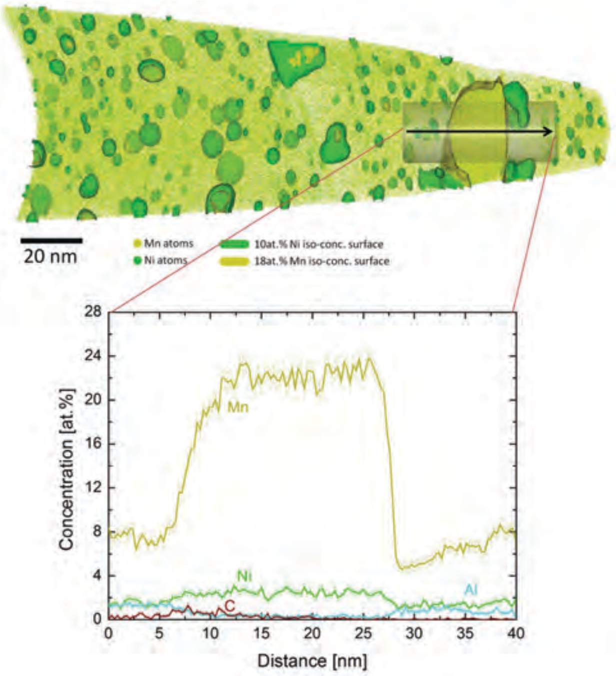


**Fig. 13:** *APT observation of the formation of Mn-rich austenite at a martensite interface in a Fe-Mn-based maraging steel (Fe–12Mn–2Ni–0.15Al–1Ti–1Mo–0.01C, wt.%) upon quenching and subsequent tempering at 450°C for 48 hours. The in-grain envelope zones in the APT map indicate intermetallic nanoparticles that form during tempering (J. Millán, D. Ponge).*

instable phases and the strain hardening effects that may result from local transformations, we observed that it is vital to design the phase stability and hence the strain hardening as a sequence of activated mechanisms that do not occur at the beginning of loading but gradually at later deformation stages, i.e. during ongoing loading at higher deformations.

Examples for successful new alloy design directions resulting from this strategy are maraging TRIP steels, TWIP– and TRIPLEX steels, Ti- and Fe-based GUM alloys, and ductile Mg.

A further essential detail pertaining to this strategy is the observation that the nanostructuring of such instable second phases leads in many cases to a profound increase in ductility without loss in strength. Examples are novel superplastic steels [88]; ultrafine grained dual phase and C-Mn steels [55,58-63]; ultrastrong maraging-TRIP steels that are rendered ductile by the stabilization of retained austenite, formation of new instable re-austenitization layers on the former martensite lath grain boundaries, and intermetallic nano-precipitates, Figs. 13,14 [1,14]; nanotwin formation in Fe–Mn–C TWIP steels [15,21]; amorphous steels containing nanocrystalline second phases; weight-reduced Fe–Mn–Al–C steels containing nano-sized kappa carbides, Fig. 12

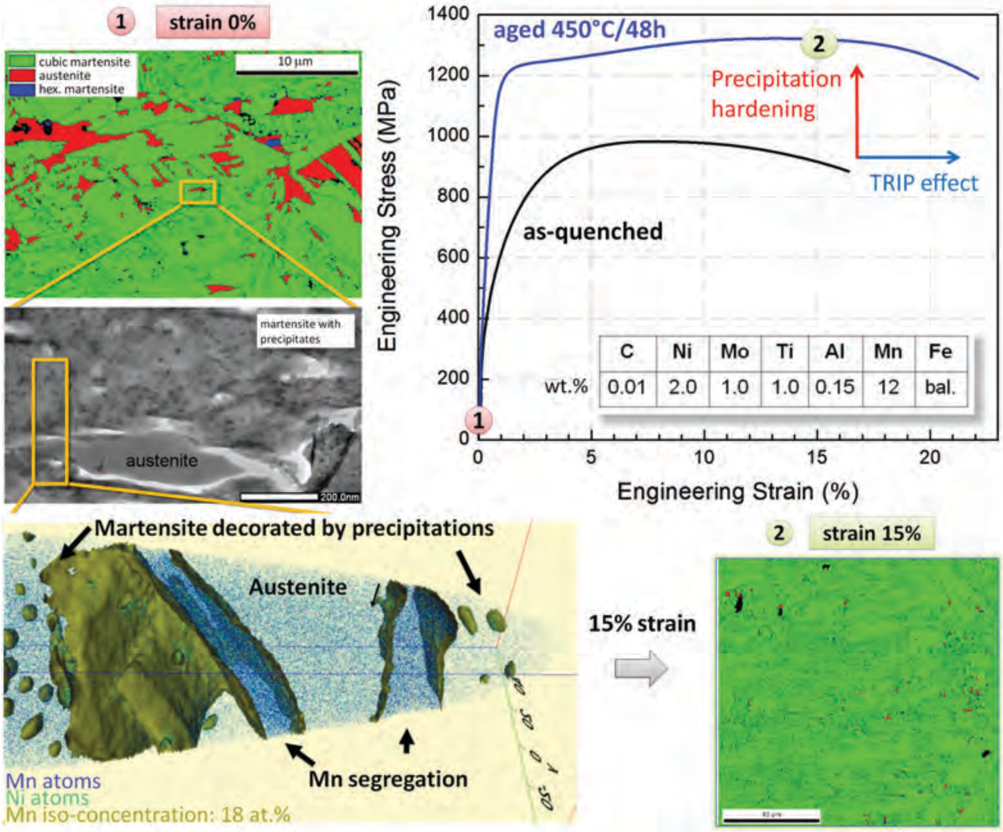


**Fig. 14:** *The stress-strain curves illustrate the increase in strength from precipitation hardening and ductility enhancement from the TRIP effect. At 0% strain (1), the electron backscatter (EBSD) phase map shows significant amounts of retained austenite. Upon 15% straining (2), the retained austenite disappears in an EBSD phase map taken at the same magnification. The atom probe tomography analysis shows nanoparticles inside the martensite matrix and precipitate-free austenite regions. The Mn enriched layers (up to 27 at.%) at the interfaces between austenite and martensite is due to partitioning, subsequent austenite reversion, and kinetic freezing of Mn in the interface region [1,37,38].*

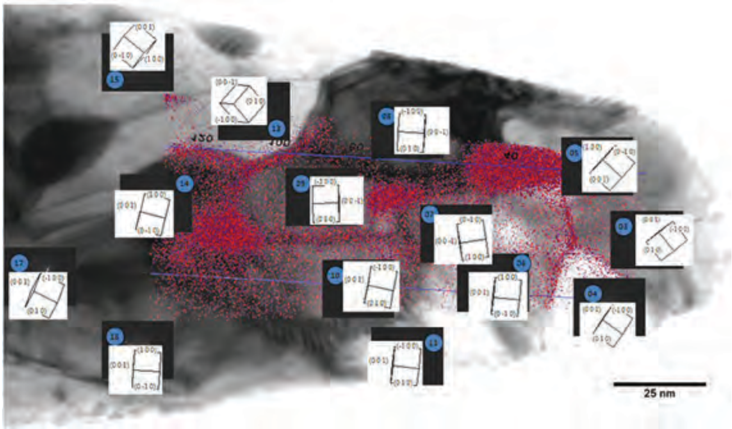


**Fig. 15:** *Joint determination of the crystallographic orientation of the carbon-decorated subgrains (carbon atoms in red) and their chemical composition in pearlitic ferrite by TEM diffraction and APT (6.02 GPa UTS cold-drawn Pearlite -> annealed for 2 minutes at 400°C) (M. Herbig, Y.J. Li, P. Choi, S. Goto, D. Raabe, R. Kirchheim).*

[39]; and nanostructured pearlite [41-43], Fig. 15. Regarding the latter material we currently hold the record of the world's strongest bulk structural alloy having a yield strength of about 6.3 GPa [43].

## II. New insights: Advanced characterization of complex materials

The second field of long term developments is the development of a sequence of characterization methods that matches the hierarchy inherent in complex metallic micro- and nanostructures. This means that we require adequate structure and composition mapping at all scales that matter for understanding and quantifying the lattice defect populations that lead to the desired mechanical properties addressed above.

Mesoscopic characterization of the chemical and microstructural homogeneity of cast, formed, and heat treated samples can be conducted by using optical and scanning electron microscopy (SEM) in conjunction with EDX (energy dispersive x-ray spectrometry) and high resolution EBSD (electron back scatter diffraction). As suited SEM for this purpose we usually use a JEOL JSM-6500F field emission scanning electron microscope (FE-SEM) operated at 15 kV. The EBSD scans can be carried out in large areas or at high resolution down to a step size of 40 nm for the determination of phase patterning. When the 3D topology of the second phases is of high relevance 3D EBSD can also be used. This device consists of a dual beam set-up where we use fully automated serial sectioning and EBSD scanning cycles to reconstruct the microstructures in full 3D (see p. 117).

Strain-hardening phenomena in crystalline metallic act essentially through the reduction of the dislocation mean free path, for instance, through smaller grain sizes (UFG), mechanical twins (TWIP), cell walls, or phase transformations (TRIP). All these additional interfaces act as obstacles to dislocation glide. Mechanical twins in TWIP steels are extremely thin, and hence are generally studied by transmission electron microscopy (TEM). However, TEM is limited when it comes to the quantitative characterization of highly heterogeneous microstructures, such as encountered in deformed TWIP steels. Another microscopy technique for characterizing deformed microstructures is electron channeling contrast imaging (ECCI). ECCI is a scanning electron microscopy (SEM) technique that makes use of the fact that the backscattered electron intensity is strongly dependent on the orientation of the crystal lattice planes with respect to the incident electron beam due to the electron channeling mechanism [15,21,22]. Slight local distortions in the crystal lattice due to dislocations cause a modulation of the backscattered electron intensity, allowing the defect to be imaged. For quantitative characterization of dislocation structures (e.g. Burgers vector analysis) and to image these structures with optimal contrast, it is required to conduct ECCI under well-controlled diffraction conditions as dislocation imaging is obtained by orienting the crystal matrix exactly into Bragg condition for a selected set of diffracting lattice planes. To date the only method that was utilized for performing ECCI of dislocations under controlled diffraction conditions is based on electron channeling patterns (ECPs). The drawback of this technique is the requirement of a large final aperture to allow the beam to cover a large angular regime, leading to very low spatial resolution which is almost two orders of magnitude above the resolution of EBSD. This shortcoming reduces its application to the imaging of dislocation structures in lightly deformed metals. This also explains the limited number of works on the use of ECCI for imaging dislocation structures. In the past years we have developed a novel set-up for the ECCI technique under controlled diffraction conditions where the crystal orientation is obtained by means of EBSD. This set-up provides an efficient and fast means to perform ECCI of dislocations under controlled diffraction conditions with enhanced dislocation and interface contrast [15,21,22], Figs. 6,7,9.

When higher resolutions are required for nano-structure analysis, transmission electron microscopy (TEM) is applied. For TEM sample preparation the material is usually first thinned to a thickness below 100 µm by mechanical polishing. Standard 3-mm TEM discs are then punched and electropolished into TEM thin foils using a Struers Tenupol twin-jet electropolishing device. The electrolyte typically consists of 5% perchloric acid ($HClO_4$) in 95% ethanol cooled to −30°C. Alternatively FIB thinning is possible too using our FEI nanolab dual beam system. The thinned specimens can then be investigated in the field emission transmission electron microscope JEOL JEM 2200 FS operated at 200 kV. The analysis are usually carried out in scanning TEM mode (STEM) using a bright field (BF) detector.

For yet higher resolution, specifically regarding the local chemical composition, nanostructure characterization via atom probe tomography (APT) is conducted. APT characterization is highly suited to better understand nanostructural changes in non-equilibrium alloys such as addressed by our group [1,9]. Its results can be compared to *ab initio* or conventional thermodynamic predictions regarding chemical phase composition or partitioning. APT characterization is carried out using a state-of-the-art local electrode atom probe. This instrument provides three-dimensional elemental maps in real space with a maximum field of view of 200 nm. Both, structural and spatially resolved chemical analyses can be realized with sub-nanometer resolution. Special features of the installed instrument are a wide-angle reflectron, which enables high mass resolution (and therefore the analysis of multi-component alloys and detection of low elemental concentrations) and an ultrafast laser, which allows for the analysis of non- and semi-conducting materials. By applying high-resolution electron microscopy as a complementary technique, we are capable of identifying not only the thermodynamic and compositional but also the structural information at near atomic resolution, Fig. 16.

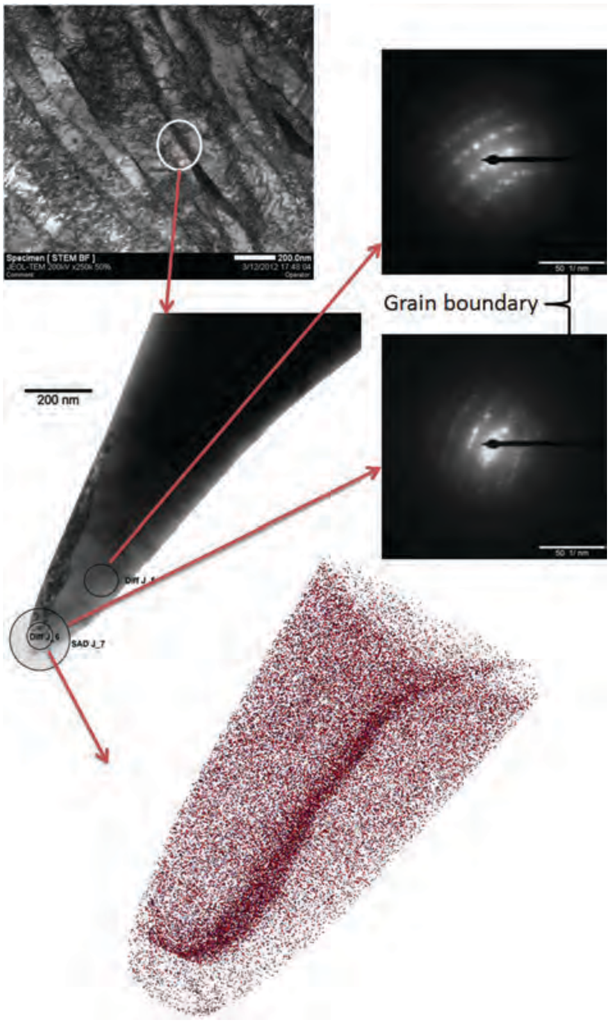


***Fig. 16.*** *Example of a site specific joint STEM-APT analysis of a grain boundary in a Fe–C–Mn martensite alloy. The dots indicate the positions of carbon atoms as measured by atom probe tomography. The joint analysis reveals strong segregation of carbon at the lath martensite grain boundary. The misorientation of this lath martensite interface amounts to about 7°. The depth of the evaporated volume is approximately 180 nm (M. Kuzmina, D. Ponge).*

## III. New predictions: Multiscale models for quantitative simulations

For the alloy design strategy outlined above the prediction of accurate phase diagrams and of non-equilibrium phase transformations is a key element. While equilibrium data for stable phases are straightforward to measure and thus commonly available with high precision it is principally impossible to synthesize unstable bulk phases. Deducing their thermodynamic or mechanical properties is therefore only indirectly possible by e.g. epitaxially stabilizing such phases on suitable surface substrates (restricted to thin films only) or by extrapolating from the stable regime into the unstable one. In both cases the practical applicability is limited, often requires complex and expensive experimental setups, and provides large and often hard to estimate error bars. *Ab initio* calculations as a basis for searching unstable phases such as conducted on the department of J. Neugebauer is hence the basis and starting point for corresponding multiscale simulations of corresponding strain hardening phenomena that are based on non-equilibrium transformations (e.g. in TRIP, TWIP or GUM steels) [1,3].

To overcome the gap between the scale that is accessible to corresponding *ab initio* calculations predicting for instance phase stability, these data must enter into mechanism-based strain hardening models at the lattice defect scale. Examples are the use of *ab initio* calculated stacking fault energy values in a Fe–Mn steel that enter as an activation barrier into the cross slip term of a dislocation rate model or into the activation stress of a mechanical twinning event. Such multiscale approaches are often not restricted to bridging length scales but equally important to bridge time scales or sampling high dimensional configuration spaces.

Important examples from the past 6 years where such hierarchical scale-bridging concepts were realized in cooperation projects between our department and that of J. Neugebauer were the prediction of elastic constants of polycrystals by combining single crystal *ab initio* calculated elastic tensors with homogenization concepts developed in theoretical mechanics; the brittle-to-ductile transition behavior of Mg–Li alloys over the entire composition range; the activation of mechanical twinning in TWIP steels as a function of chemical composition and stress levels (Fig. 6); the prediction of B2 and Heusler-type nano-particles in maraging steels, Figs. 13,14 (see p. 101), and Ti-based instable BCC and related Gum alloys which are characterized by large plastic yet hardening-free deformations (see p. 113). Further details about some of the developed multiscale concepts were part of the last bi-annual report.

## Spirit and Outreach

Projects within our group and also among the departments are pursued in an interdisciplinary and team-oriented spirit. Scientists in our department come from such different backgrounds as metallurgy, physics, materials science, mechanical engineering, informatics, chemistry, and biology. Projects are conducted in an atmosphere of mutual inspiration, respect, communication, and cooperation. Paramount to the success of our work is the close exchange among theorists and experimentalists and an open minded attitude among the different disciplines.

The working atmosphere was during the past years dominated by an international flair bringing together young scientists and visiting scholars from Argentina, Australia, Bangladesh, Belgium, Brazil, Bulgaria, Colombia, China, Egypt, France, Germany, India, Indonesia, Iran, Japan, Jordan, Korea, Mexico, Nigeria, Romania, Russia, Sweden, Spain, Ukraine, Poland, The Netherlands, Turkey, UK, Ukraine, USA, and Venezuela. Our international orientation is also reflected by our extramural cooperation partners, namely, Prof. Schneider, Prof. Bleck, Prof. Mayer, Prof. Friedrich, and Prof. Gottstein (RWTH Aachen, Germany), Prof. Dunin-Borkowski (Ernst Ruska-Centre, Research Centre Jülich, Germany), Prof. Rollett and Prof. Rohrer (Carnegie Mellon University, USA), Prof. Lebensohn (Los Alamos, USA), Prof. Radovitzky (MIT, USA), Prof. Mao (University of Science and Technology Beijing, China), Prof. Sandim (University of Lorena, Brazil), Prof. Bieler and Prof. Crimp (Michigan State University, USA), Prof. Mason (Albion College, USA), Prof. Hono and Prof. Adachi (National Institute for Materials Science, Japan), and Prof. Kobayashi (Tohoku University, Japan).

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## Research Projects in Progress

### Microstructure and Alloy Design (D. Raabe)

*Khorashadizadeh, Raabe*: Deformation-induced orientation laminates and orientation patterning in single- and polycrystals

*Raabe, Gutierrez, Zaefferer*: Fundamentals of soft magnetic Fe–Si transformer steels

*Sandlöbes, A. Eisenlohr, Raabe*: Microstructure and mechanical properties of Mg–Li alloys

*Sandlöbes*: Synthesis and Characterization of Fe-Mn reference materials

*Sandlöbes*: Constitutive modelling and microstructural validation for crystal plasticity finite element computation of cyclic plasticity in fatigue

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

### Theory and Simulation (F. Roters)

*Eisenlohr, Roters*: Development of a scale bridging method for describing deformation and intercrystalline fracture in Molybdenum

*Eisenlohr, Roters, Bieler, Crimp, Raabe*: Physically based approach for predicting and minimizing damage nucleation in metals

*Raabe, Roters, Tasan, Diehl, Eisenlohr*: Simulation of the mechanical response of stable dualphase steels

*Roters, Eisenlohr*: Materials World Network: Physically based approach for predicting an minimizing damage nucleation in metals

*Steinmetz, Zaefferer, Raabe, Roters, Eisenlohr*: Twinning mechanism in Mn TWIP steels

### Diffraction and Microscopy (S. Zaefferer)

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

*Gutierrez, Zaefferer, Raabe*: Local mechanical textures and properties of Mn-based steels

*Jäpel, Zaefferer*: Local strain determination in Mn-based steels

*Khorashadizadeh, Raabe, Zaefferer*: 5D Grain boundary characterization in ultrafine grained Cu–Zr alloys

*Sandlöbes, Zaefferer*: Fundamental investigation of the mechanisms of deformation and recrystallisation of cold deformable Mg alloys microalloyed with rare earth elements and microstructure optimization for the development of a new class of Mg alloys

*Steinmetz, Zaefferer, Raabe*: High resolution scanning electron back scatter diffraction experiments

*Zaefferer*: *Insitu* SEManalysis and internal stress determination of threepoint bending tests

*Zaefferer, Elhami*: Characterization of the microstructure and deformation mechanisms in TWIP(XIP u. LIP) steels

*Zaefferer, Raabe*: Local textures and anisotropy in Mn-steels

### Alloy Design and Thermomechanical Processing (D. Ponge)

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

*Ponge, Springer, Raabe*: Bladestrip - Innovative material production for blades and cutlery by strip cast technology

*Raabe, Ponge, Millan, Springer*: Mechanics of grain- and phase boundaries in multiphase steels

### Biological Materials (H. Fabritius)

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

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

*Raabe, Fabritius*: Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials

*Raabe, Fabritius*: Crustacean skeletal elements: variations in the constructional morphology at different hierarchical levels

### Atom Probe Tomography (P. Choi)

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

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

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

*Cojocaru-Mirédin, Raabe*: Optimization of solar cells efficiency based on 3-dimensional chemical analysis at atomic-scale

*Jägle, Choi, Raabe, Hickel, Neugebauer*: Atomic scale investigation of the kinetics of nano-precipitation in Fe–Si–Cu alloys using atom probe tomography and *ab initio* informed Monte Carlo methods

*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

*Raabe, Schneider, Choi*: Topological Engineering of Ultra-Strong Glasses

### Computational Mechanics of Polycrystals (P. Eisenlohr)

*Eisenlohr, Roters*: Development of a scale bridging method for describing deformation and intercrystalline fracture in Molybdenum

*Eisenlohr, Roters, Bieler, Crimp, Raabe*: Physically based approach for predicting and minimizing damage nucleation in metals

*Roters, Eisenlohr*: Materials World Network: Physically based approach for predicting an minimizing damage nucleation in metals

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

### Theory and Simulation of Complex Fluids (F. Varnik)

*Varnik, Krüger, Raabe*: Experimental and theoretical investigations of the dynamics of collective phenomena in blood I: Idealized vesicle/fluid droplet models

*Varnik, Raabe*: Nonequilibrium flow at gradient surfaces: multicomponent fluids

### Combinatorial Metallurgy and Processing (H. Springer)

*Ponge, Raabe, Springer, Belde, Yuan*: Microstructure, austenite reversion and forming properties of martensitic Cr steels

*Ponge, Springer, Raabe*: Bladestrip - Innovative material production for blades and cutlery by strip cast technology

### Adaptive Structural Materials (C. Tasan, B. Grabowski CM Dept.)

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

# Department of Structure and Nano-/Micromechanics of Materials

*G. Dehm*

## Introduction

Gerhard Dehm and three of his PhD students moved from the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences and the Department Materials Physics of the University Leoben to MPIE on 1st of October 2012. The newly formed department will be structured in 5 scientific groups working in the field of

- Nano-/Micromechanics of Materials,
- Advanced Microstructure Characterization,
- Nanotribology,
- Synthesis of Nanostructured Materials,
- Intermetallics.

All 5 groups will be interlinked to understand the mechanical response of materials focusing on small length scales by applying novel nano-/micromechanical approaches combined with advanced microstructure characterization techniques. The gained knowledge will be used to develop and improve nanostructured and intermetallic materials. Currently, most positions of the group leaders are vacant except for the already established scientific group Intermetallics which is headed by Dr. Martin Palm and Dr. Frank Stein. For the research group Nano-/Micromechanics of Materials a group leader has been identified and will start with 1st of March 2013.

The newly formed department needs dedicated laboratories space especially for the installation of an advanced transmission electron microscopy (TEM) facility. This facility will open new horizons for *in situ* studies of dynamic material processes, atomic structure investigations and chemical analysis at ultra-high spatial resolution for structural and functional materials and expands the already existing conventional TEM laboratory. The advanced TEM facility will be located in hall 8 and 9 which must be adapted to host all TEMs of MPIE and the corresponding infrastructure for sample preparation and analysis by metallography methods, optical microscopy, scanning electron microscopy and focussed ion beam microscopy. The planning of the reconstruction work of hall 8 and 9 has already started and the remodeled laboratories are expected to be available in fall 2014.

**Fig. 1:** *First group picture of the newly formed department Structure and Nano-/Micromechanics of Materials taken at the beginning of October 2012.*

# Scientific Mission

Plasticity, fatigue, and fracture of materials are usually initiated by local deformation processes. Detecting and understanding the underlying mechanisms is the key to improve the mechanical performance and lifetime of **miniaturized materials** and also of **macroscopic materials**. Many **advanced structural materials** possess complex multiphase microstructures where the mechanical interplay of the different phases and their interfaces is poorly understood. Similarly, **functional materials** employed in modern micro- and nano-technologies are composed of material stacks and/or of different phases and possess confined geometries such as thin films, lines, rods, etc.. Such micro- or nano-sized materials often show a completely different mechanical performance compared to their bulk counterparts as a consequence of confinement effects. The **mission** of the Department Structure and Nano-/Micromechanics is

- to develop experimental methods to perform **quantitative nano-/micromechanical** and **tribological** tests for complex and miniaturized materials,
- to unravel the underlying deformation mechanisms by **advanced microstructure characterization** techniques from the micrometer level down to atomic dimensions,
- to establish **material laws for local and global mechanical behavior**, and finally
- to generate **nanostructured materials** and high temperature **intermetallic materials** with superior mechanical properties.

The in-depth microstructure investigations include atomic resolved high-resolution TEM, analytical and conventional TEM, scanning electron microscopy with electron backscattered diffraction (SEM/EBSD), focussed ion beam microscopy (FIB), X-ray diffraction and synchrotron radiation techniques. A cornerstone will be the combination of advanced characterization and mechanical testing in form of *in situ* nano-/micromechanical experiments which will permit to simultaneously observe the microstructural changes while measuring the mechanical response. The gained insights will be used to quantitatively describe and predict the local and global material behavior and to design superior nanostructured materials and high temperature intermetallic materials by using local confinement effects. The synthesis of miniaturized nanostructured materials will be done by molecular beam epitaxy.

# Scientific Concepts

The research work in the department **Structure and Nano-/Micromechanics of Materials** will focus on:

1. Development and application of novel nano-/micromechanical methods on bulk and miniaturized materials to study mechanical effects at small length scales.
2. Characterization of the microstructure and dynamic microstructural processes by advanced transmission electron microscopy methods, scanning electron and ion beam microscopy, and advanced X-ray techniques including synchrotron radiation.
3. Developing concepts to study nanotribology at metallic surfaces and to understand the processes of wear.
4. Synthesis of nanostructured materials and model systems by using molecular beam epitaxy.
5. Study of the structures, phase stabilities and phase transformations of intermetallic phases as a basis for the development of novel materials.

The research objectives in these five fields are summarized below.

1. In area 1 experimental approaches to study deformation phenomena at small length scales are developed and employed. The materials of interest are small scale materials as used in microelectronic and information technology as well as bulk structural and functional materials. Topics of interest are: onset of plasticity, length scale aspects of plasticity („size-effects“), brittle to ductile transitions especially in intermetallic materials, semiconductors, and ceramics, fracture behavior, crack growth and crack shielding phenomena, etc. The experiments will be conducted at different temperatures and under different environment (vacuum, $N_2$, etc.). Basic

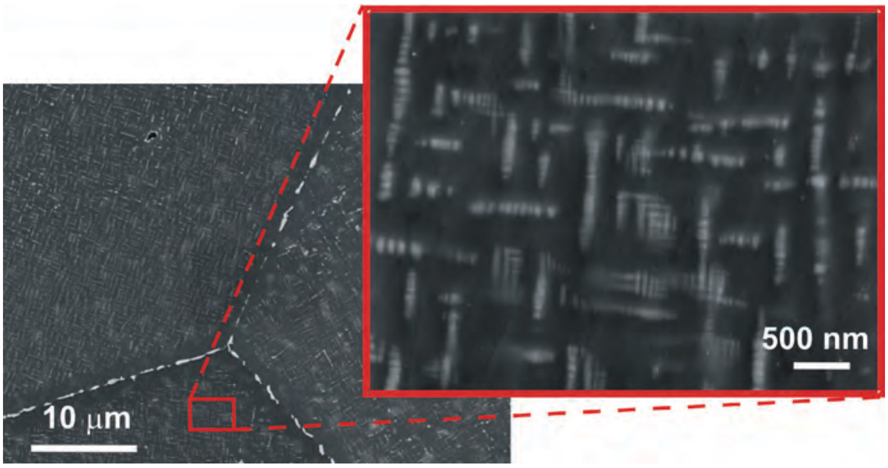

**Fig. 2:** *SEM and high-resolution SEM micrographs of a novel Fe$_3$Al-based alloy, strengthened by chains of coherent, nm-sized precipitates of Fe$_2$AlTa Heusler phase.*

insights in the mechanical behavior of miniaturized materials and local material properties of bulk materials are the main task. This information may provide basic understanding of length-scale effects which in turn can be used for materials design concepts. Modelling of the mechanical phenomena will be done in close collaboration with the departments MA and CM, while environmental and chemical effects will be studied in collaboration with the department GO.

2. This area complements area 1 and provides the experimental methods to analyze the microstructure in advanced materials (Fig. 2) and their change during mechanical loading. One of the major methods will be *post mortem* and *in situ* TEM characterization to analyze the dominating deformation mechanisms related to micro-/nanomechanical materials response. In addition, the basic mechanisms in interface dominated materials and phase transformations will be studied. This includes transitions from interface sliding to interface fracture for heterophase boundaries exposed to deformation at different temperatures as well as size effects (confinement effects) in phase transformations of materials. Other possible questions involve ion exchange at interfaces, interface strain, and mechanical consequences. A technique which will be implemented as well in this area is X-ray diffraction (in-house laboratory and synchrotron radiation). Structures of interfaces determined by atomic resolved TEM investigations will be linked to atomistic calculations performed in the department CM. Similarly, chemical analysis by atom probe tomography and advanced EBSD techniques carried out in collaboration with the department MA will complement the research efforts of this area.

3. Materials are frequently in sliding contact with counterparts. This leads to friction and wear effects. While some basic concepts such as the Amontons-Coulomb Law and the stick-slip behavior are established, microstructural mechanisms which in turn lead to severe microstructural modifications in a surface zone are not yet fully understood. E.g. single crystal metals in sliding contact with a ceramic will develop a nanostructured zone with a very fine grain size. Understanding the underlying phenomena will open a link between tribology and microstructure for predicting materials behavior under sliding contact. Important parameters which will be studied include the influence of temperature and environment (liquid, dry, humidity, …). Materials of interest stretch from structural materials, thin film systems, to selected biological materials. Cross-sections will be made using ion beam microscopy and studied using advanced microstructure characterization techniques including advanced TEM and X-ray diffraction methods. Close links to the department GO, MA, and CM are anticipated for the research area nanotribology to gain a basic understanding of chemical and structural changes in the surface-near zone.

4. Thin film deposition techniques are one way to produce nanostructured materials. Initially the focus will be laid on molecular beam epitaxy (MBE) of mainly metallic films and nanostructured metals. The systems which will be investigated include metal-polymer systems, well defined multilayers, nano-composite film structures, and growth of nanorods. Additionally, research in this area will include studies on metastable microstructures. Questions to be addressed are minimum grain size in nano-composites, evolution of nanostructures in non-equilibrium condi-

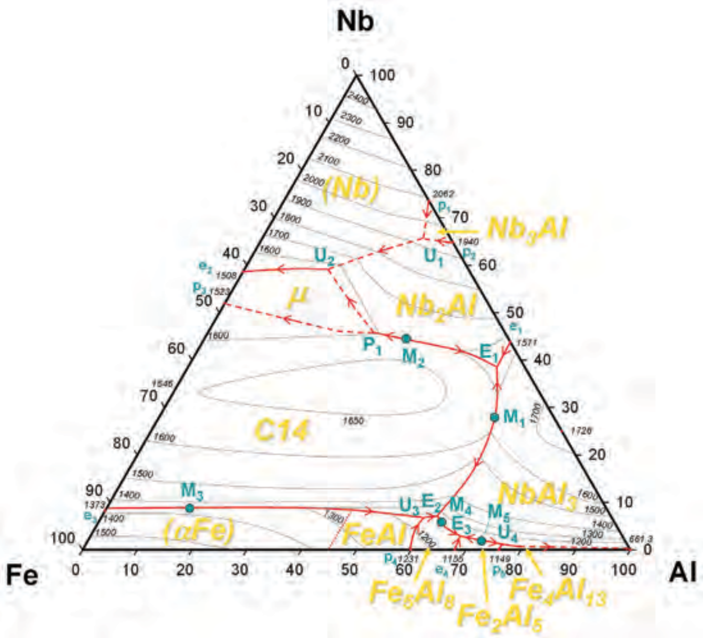

**Fig. 3:** *Liquidus surface of the Fe–Al–Nb system as obtained from a combination of differential thermal analysis, scanning electron microscopy, electron probe microanalysis and X-ray diffraction.*

tions exceeding solubility limits, and stabilization of metastable phases. This topic provides strong links to all three departments at the MPIE.

5. Materials based on intermetallic phases comprise a new class of materials entering into application, e.g. TiAl compressor blades in the new $GE_{NX}^{TM}$ jet engines. The basis for any new material development is a sound understanding of the stability of the constituting phases in dependence of composition, temperature and time, i.e. knowledge of the respective phase diagrams. The structures, phase stabilities and phase transformations of intermetallic phases are therefore studied by microscopy, X-ray diffraction, electron probe microanalysis and differential thermal analysis, among others. The results – often combined with CALPHAD modeling – are used to establish phase diagrams, isothermal sections and liquidus projections (Fig. 3). These are further on employed for the development of novel materials. Current activities focus on Laves phases, Al-rich Ti–Al (c.f. p. 109) and Fe–Al intermetallic phases. All of the above topics, but specifically the basic mechanical properties of the intermetallic materials and their underlying phenomena, are studied in close connection with the other groups of the department. Further cooperation with all other departments exists, e.g. currently on rolling (MA), corrosion in steam (GO) and environmental embrittlement (CM) of Fe–Al based materials.

# Max Planck Fellow Research Group on High Temperature Materials

*A. Kostka, G. Eggeler*

High temperature materials are an important material class for energy conversion and transportation. They represent a fascinating subject area for research in different fields of materials science and engineering. High temperature materials are usually difficult to process and manufacture. They generally have complex microstructures and, therefore, a good understanding of thermodynamic stability and microstructural evolution during high temperature exposure is required.

In the High Temperature Materials Group (HTM) we take a broad view on materials science and engineering of high temperature materials focusing on interesting physical, chemical, microstructural and mechanical topics. We presently work on (1) elementary dislocation processes during high temperature and low stress creep of Ni-based single crystal superalloys, (2) the evolution of microstructure in 9-12% Cr tempered martensite ferritic steels (TMFS) during long term creep exposure, (3) the effects of grain boundary crystallography and chemistry on creep cavity nucleation and growth, and (4) the characterization of interfacial regions which form during joining of dissimilar materials due to multi atom interdiffusion processes. In the following we present three examples for the type of research performed in HTM.

The first example relates to our work in the field of Ni-based single crystal superalloys. Fig. 1 compiles scanning electron microscopy (SEM) and transmission electron microscopy (TEM) micrographs of important microstructural features that characterize these materials.

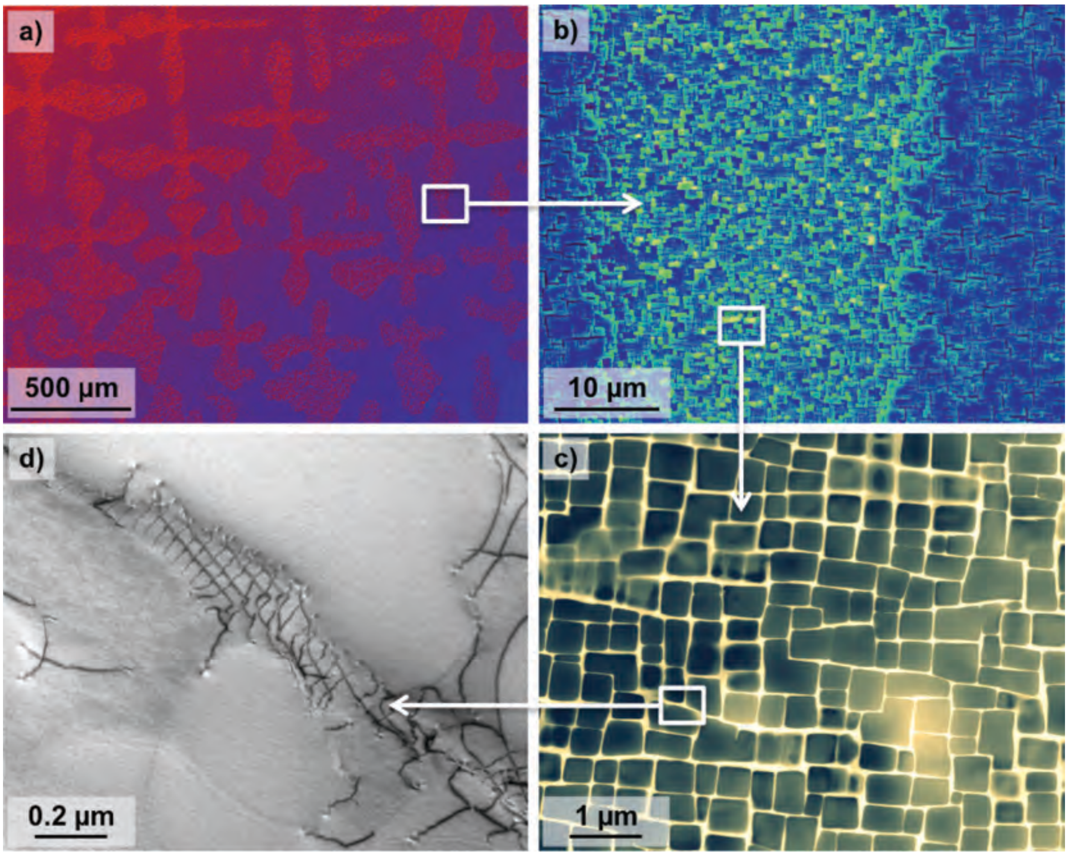

**Fig. 1:** *Micrographs showing characteristic features of single crystal Ni-base superalloys. (a) SEM micrograph in the [001] cut revealing arrangement of dendrites. (b) SEM micrograph showing the transition between former dendritic and interdendric regions. (c) TEM micrograph of γ/γ'-microstructure. (d) TEM micrograph showing dislocations in γ-channels of the γ/γ'-microstructure.*

**Fig. 2:** *Participants of the first SFB/Transregio 103 interaction week, Erlangen June 2012.*

Performing research on single crystal superalloys with the types of microstructures shown in Fig. 1, HTM links MPIE research activities to the interdisciplinary research in the new collaborative research center SFB/TR 103, where single crystal super alloys are in the focus of interest. They represent key materials for turbine blades in modern gas turbines for aero engines and power plants. Worldwide air transportation and global energy production rely on this fascinating class of high temperature materials. Improvements in efficiency and emissions demand new concepts in single crystal technology, which require progress in four areas of expertise: (1) Basic understanding of all aspects associated with alloy composition / microstructure design and creep performance: microstructural instability during creep, elementary deformation and damage process during creep, dislocation reactions in single crystal Ni-based superalloys. (2) The continuous improvement and innovation of processing technologies for establishing specific nano- and microstructures with better homogeneity, improved creep and corrosion resistance (single crystalline solidification in a ionic liquid cooling bath, additive processing using selective electron beam melting, heat treatments under hydrostatic pressure, and coating technologies). (3) We pursue obtaining better knowledge of materials properties and microstructure through the use of improved testing procedures, either by mechanical measurements such as miniaturized creep and fatigue testing or by the use of latest high resolution characterization methods (high resolution, aberration corrected transmission electron microscopy, 3D atom probe). (4) Materials modeling bridging all scales, from atomistic (*ab initio* methods, molecular dynamics) to mesoscopic (discrete dislocation modeling and thermodynamic / kinetic modeling of microstructural evolution) and macroscopic (physically sound constitutive equations). Modeling is to be applied to materials processing as well as high temperature behavior.

In addition to the SEM and TEM type of work as shown in Fig. 1, MPIE brings in expertise on the 3D atom probe method (Dr. P. Choi and Dr. I. Povstugar) that allows chemical analyse of 1 $\mu m^3$ volumes to study elementary diffusion reactions in high temperature materials. In SFB/TR 103, HTM provides a detailed microstructural characterization of materials in the initial state and after well-defined creep periods. We explore the role of small and large-scale microstructural heterogeneities, provide quantitative data on porosity, dendritic structure and the evolution of the $\gamma/\gamma'$-microstructure. We focus on the elementary processes that govern the high temperature deformation of these materials. MPIE researchers participated in the first interaction week organized in Erlangen in May 2012 in the framework of SFB/TR 103, Fig. 2.

The second example of work performed within HTM considers the elementary processes (nucleation, growth kinetics, evolution) governing the formation of transition zones during high temperature joining of dissimilar materials. More specifically, the project focuses on the formation of intermetallic phases that form in the Fe−Al system during laser beam welding of iron to aluminium. The low density and good corrosion resistance of aluminum combined

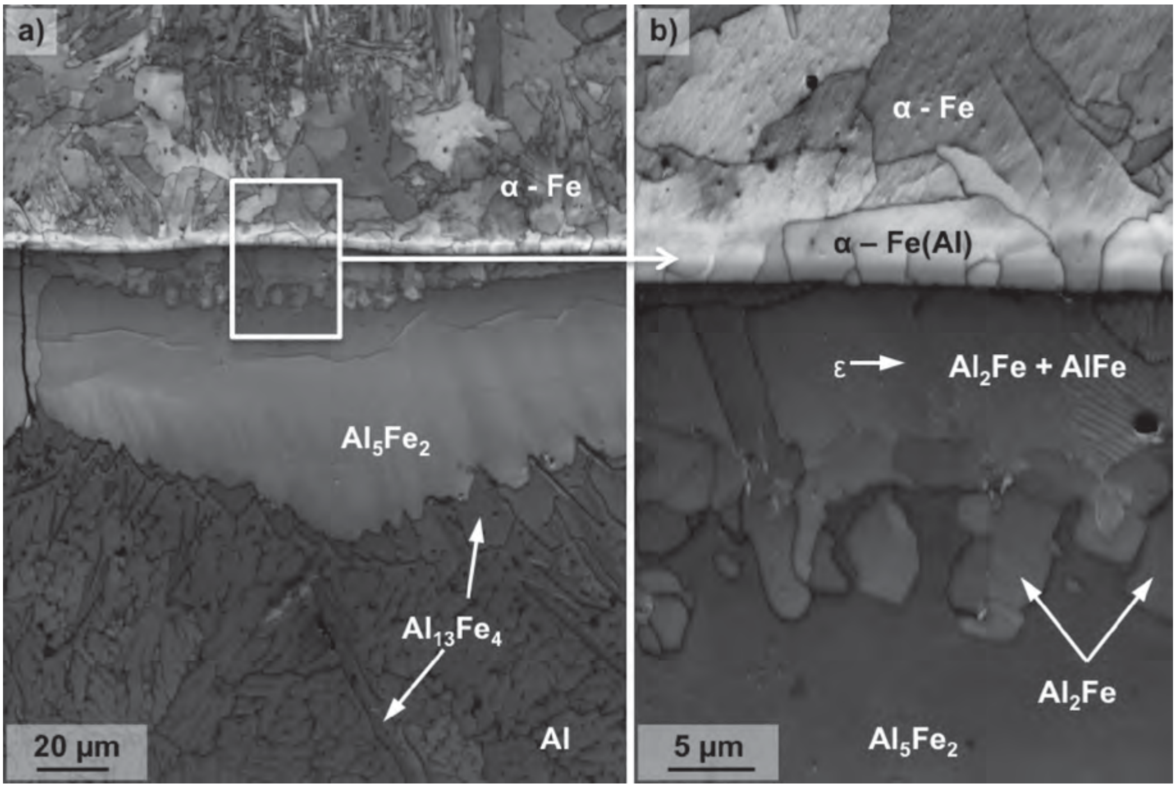

**Fig. 3:** *EBSD quality maps from transition regions formed during laser welding of low carbon steel to aluminium. (a) Fast growth of the* $Al_5Fe_2$ *- phase in the direction perpendicular to the steel/aluminum interface. (b) Formation of new intermetallic phases between the steel and* $Al_5Fe_2$ *layer (DFG: KO 3998/1-1).*

with the high strength and good formability of steel provides a highly versatile compound for engineering structural applications. Since Al-rich phases that typically appear in the Al–Fe system are extremely brittle, optimization of the joining process parameters which control the thickness of intermetallic layers are important. The main objective of HTM's work is to contribute to a better understanding of processes that govern the metallurgical reactions which occur when solid Fe/steel and liquid Al come in contact. Especially, the thermodynamic and kintetics of the formation and evolution of intermetallic compounds like $Al_5Fe_2$ and $Al_{13}Fe_4$ are in the focus of interest. During laser welding, only the Al is liquid while the steel plate remains solid. Rapid heating, cooling and associated temperature gradients at the solid steel plate/liquid Al interface dramatically affect the composition and morphology of the reaction compounds. Moreover, local temperature gradients result in the formation of new phases, as illustrated in Fig. 3.

As a third example, we present some results which were obtained in a project that focusses on the stability of phases in tempered martensite ferritic steels (TMFS) subjected to a long term creep exposure. The project aims at understanding the nature of microstructural evolution resulting from long-term creep of TMFS at temperatures up to 600°C. The identification of the elementary processes that govern nucleation and growth of the Laves phase in TMFS is the main main scientific objective of the project. Formation of the Laves phase in TMFS occurs after long-term creep and has so far not yet been clearly understood. Its appearance may well downgrade mechanical properties. Our goal in this project can only be achieved by combining analytical transmission electron microscopy with a detailed analysis of chemical composition by atom probe analysis.

In the research on tempered martensite ferritic steels, detailed investigations of the evolution of grain boundaries and precipitates such as $M_{23}C_6$, VN, and the $Fe_2Mo$ Laves phase after different stages of creep also need to be performed by using scanning electron microscopy (OIM analysis) and transmission electron microscopy, where several techniques are applied for collecting micrographs (BF, DF, HAADF STEM, EFTEM), diffraction analysis (SAD, NBD) and chemical spectra (EDS). An example is presented in Fig. 4 (see next page).

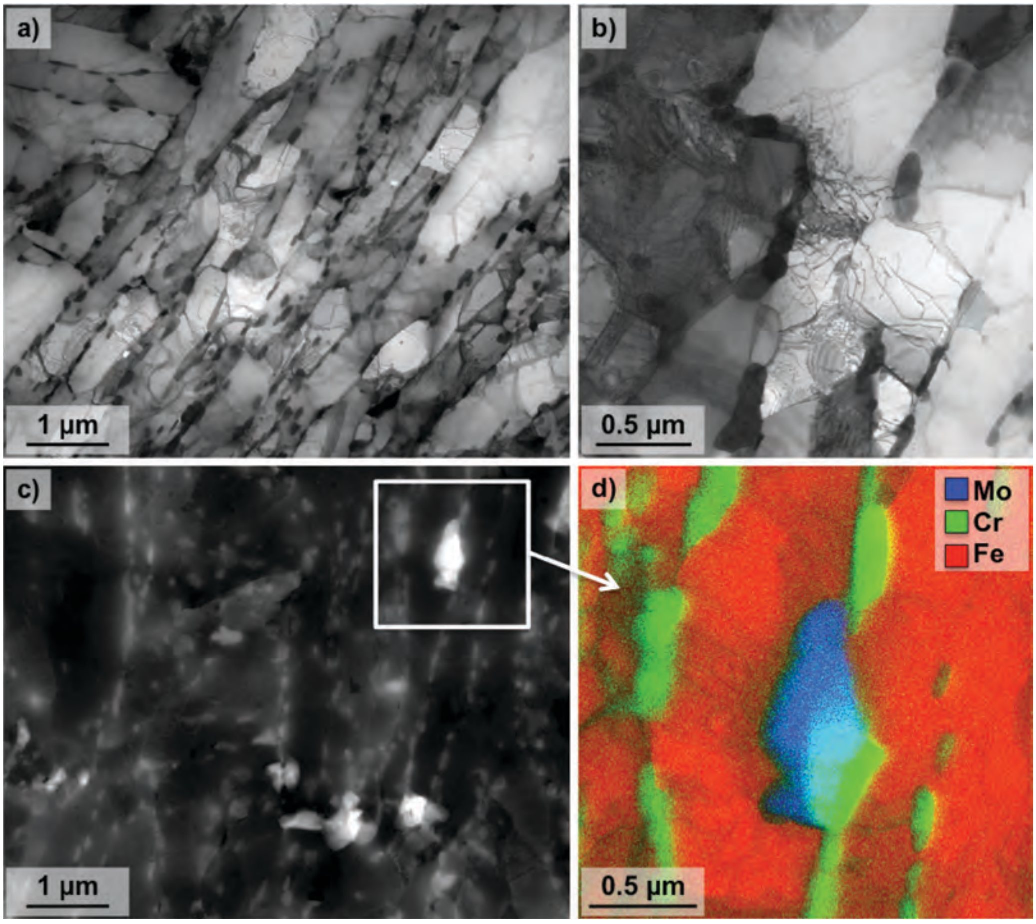

**Fig. 4:** *TEM analysis of a 12%Cr TMFS after 51000 hours creep at 650°C, 120 MPa. (a) Bright field (BF) TEM micrograph showing* $M_{23}C_6$ *carbides decorating GB's. (b) Dislocations interacting with* $M_{23}C_6$ *carbides. (c) High-angle annular dark field (HAADF) micrograph reveals particles that differ by their composition. (d) Mo, Cr and Fe element maps overlay from the highlighted region in (c) showing* $M_{23}C_6$ *carbides and formation of Mo-rich Laves phase.*

The three examples briefly introduced have in common, that non-equilibrium systems strive towards establishing an unknown thermodynamic equilibrium. Thermal activation allows for atomic mobility in the systems and plays a fundamental role in establishing microstructures and associated properties. The microstructure (constituent phases, particles, interfaces, defects) and related mechanical features (external and internal stresses) are important parameters that affect the reaction path towards thermodynamic equilibrium. HTM aims at stimulating research related to the science and technology of high temperature materials. HTM also promotes activities that help to develop new materials and processes which overcome limitations which currently hamper advances in high temperature technology.

## PART III.

# INTER-DEPARTMENTAL RESEARCH ACTIVITIES – SELECTED HIGHLIGHTS

# Design of Precipitation in Lean Maraging-TRIP Steels

J. Millán[1], S. Sandlöbes[1], T. Hickel[2], D. Ponge[1], P. Choi[1], J. Neugebauer[2], D. Raabe[1]

[1] Department of Microstructure Physics and Alloy Design
[2] Department of Computational Materials Design

"Maraging steels" combine ultrahigh strength and high fracture toughness by hardening an essentially carbon-free martensitic matrix with nano-sized intermetallic precipitates. Typical applications are in the fields of aircrafts and aerospace, where maraging steels meet the high requirements of minimum weight while ensuring high reliability [1]. The formation of a high volume fraction of homogeneously distributed precipitates such as $Ni_3Ti$ or $Ni_3Mo$ requires alloying with a high amount of expensive Ni, typically in the range of 18 wt.%.

Our approach is to combine a maraging treatment with Fe−Mn alloys and a significantly reduced Ni-content to obtain an alloy combining ultrahigh strength and sufficient ductility. As reported elsewhere [2] remarkable improvement of toughness and ductility in Fe-Mn alloys can be obtained via a partial re-austenitization.

Choosing a high Mn content of 6-12 wt.% allows reducing the Ni content (and if necessary other elements) and supports the formation of precipitates by providing a high supersaturation.

Possible intermetallic phases are NiMn or the Heusler phase $Ni_2MnAl$. NiMn can form with B2 and $Ni_2MnAl$ with either $L2_1$ or B2 structure. As both structures are based on the bcc lattice, coherency between matrix and particles is possible. This ensures low nucleation energy and favors a very fine distribution in the bcc matrix by homogeneous nucleation.

To design lean maraging TRIP steels, which are reinforced by these precipitates, we employ high resolution experimental characterization methods in combination with *ab initio* theoretical calculations.

The *ab initio* calculations were performed to determine the Al content that promotes the precipitation of either NiMn or $Ni_2MnAl$. To this aim we determined the lattice constants and formation enthalpies of the two competing phases, including the dependence on the individual alloying elements. Fig. 1 reveals that for incoherently incorporated precipitates (no constraints of the lattice constant, dashed line) the B2-NiMn phase is preferred up to 4.2 at.% (2.1 wt.%) Al content. In the case of coherency (lattice constant constraint to the matrix, solid line) the B2-NiMn phase is preferred up to 2.4 at.% (1.2 wt.%) Al content. At higher Al alloying the precipitation of $L2_1$-$Ni_2MnAl$ is favoured.

Based on these theoretical predictions we produced two different steels: Steel L-Al (0.01C−12Mn−2Ni−0.14Al−1Ti−1Mo wt.%) has a low Al content and steel H-Al (0.01C−12Mn−3Ni−1.28Al wt.%) an Al content above the critical value determined by the *ab initio* prediction. Both steels were homogenized, quenched and aged (450°C for 65 h).

TEM and APT analyses of the steels reveal the existence of nano-sized precipitates in the α' martensite in both alloys, Fig. 2. In the APT images iso-concentration surfaces at 10 at.% Ni are displayed in green to distinguish between matrix and precipitates. Ni and Mn atoms are shown by green and yellow dots respectively. Fe atoms are omitted in these reconstructions. Both characterization methods show that precipitates of different sizes and dispersion are formed in the different steels.

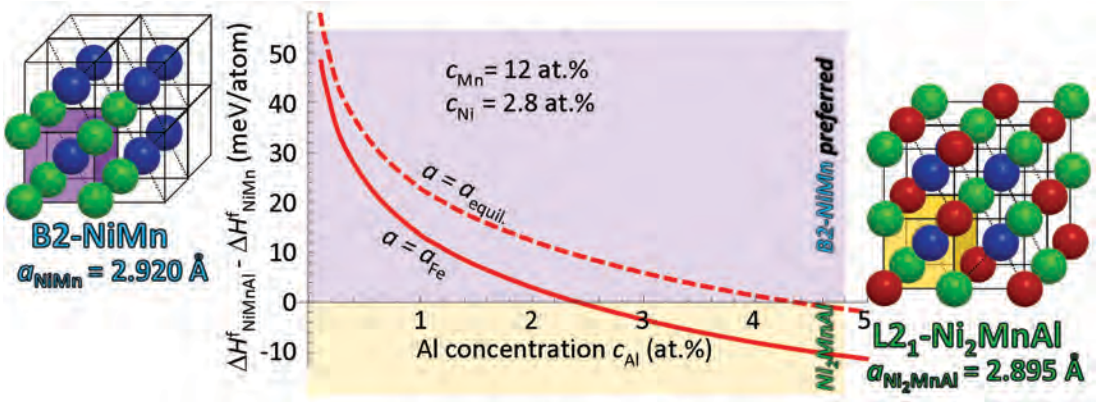

**Fig. 1:** *Difference of formation enthalpies of both phases. The concentrations of Mn and Ni are fixed, the concentration of Al is varied. Solid line: Precipitates are forced to the lattice constant of Fe (2.835 Å). Dashed line: Precipitates adopt the equilibrium lattice constants of NiMn or* $Ni_2MnAl$.

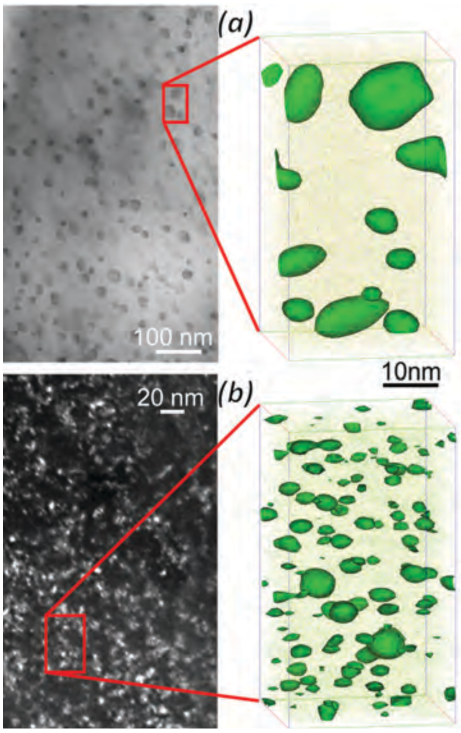

**Fig. 2:** *TEM images (left side) and APT reconstructions (right side) showing size and spatial distribution of the nano-sized precipitates in the martensitic matrix after aging at 450°C for 65 hours. (a) steel L-Al (0.14 wt.% Al), (b) steel H-Al (1.28 wt.% Al).*

In steel H-Al with higher Al content (1.28 wt.% Al) the precipitates (Ø 3-5 nm) are much finer than in steel L-Al (Ø 10-20 nm) and the number density of precipitates is 18-times higher in steel H-Al.

Selected area diffraction in the TEM investigation revealed that the structure of the precipitates in steel L-Al is B2. In contrast, in steel H-Al both structures, namely, $L2_1$ and B2 are observed.

The chemical composition of the precipitates in both steels was analyzed by APT. The average concentrations over all precipitates in the analyzed sample volumes were determined by means of the proximity histogram method. Fig. 3 shows the resulting concentration profiles between precipitates and martensitic matrix in L-Al (Fig. 3(a)), and H-Al (Fig. 3(b)). From these analyses it is evident that the precipitates have different Mn and Al concentrations: The precipitates formed in steel L-Al have an average chemical composition of 50 at.% Ni, 35 at.% Mn, 2.5 at.% Al and 5 at.% Ti. In steel H-Al precipitates with average concentrations of 50 at.% Ni, 20 at.% Mn and 20 at.% Al are formed. The stoichiometric relationships of the precipitates indicate that in L-Al NiMn particles (with substitution by Ti and Al) are precipitated, in H-Al $Ni_2MnAl$ precipitates are formed.

The combined TEM and APT analysis reveals that low Al alloying (0.14 wt.% Al in L-Al) leads to precipitation of NiMn with B2 structured precipitates and high Al alloying (1.28 wt.% Al in H-Al) yields the formation of $Ni_2MnAl$ precipitates with $L2_1$ structure as predicted by *ab initio* simulations. Hardness measurements revealed a much stronger hardening effect in the steel H-Al which contains $Ni_2MnAl$ precipitates.

We have, therefore, demonstrated that the combination of *ab initio* calculations and high resolution microstructure characterization by TEM and APT enables the design of advanced lean maraging TRIP steels with tailored properties.

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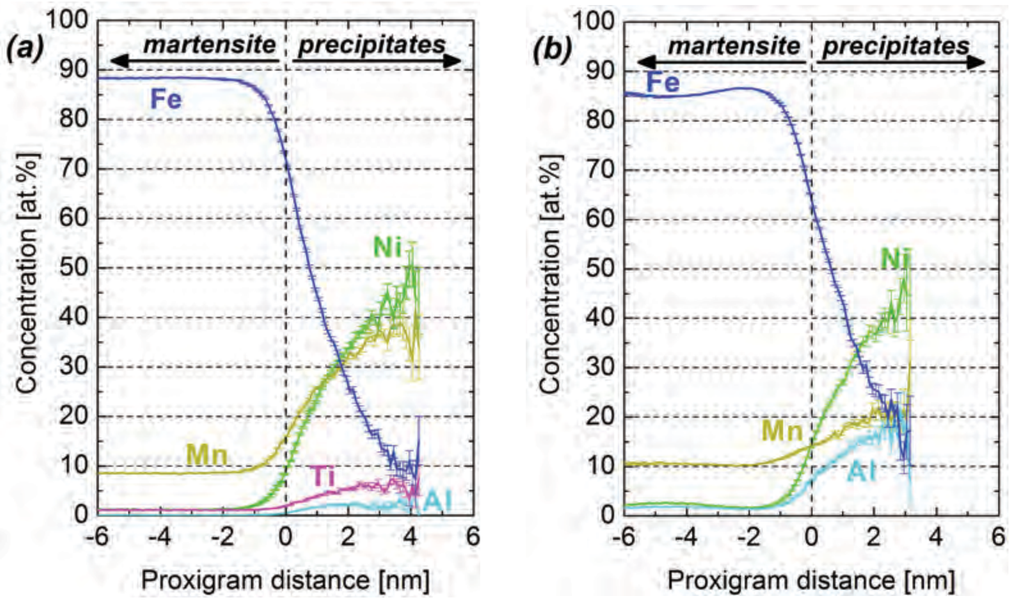

**Fig. 3:** *Average chemical composition gradients between martensitic matrix and precipitates as calculated by the proximity histogram method. Aged alloys at 450°C for 65 hours; (a) steel L-Al (0.14 wt.% Al), (b) steel H-Al (1.28 wt.% Al).*

# Scale-Bridging Analysis and Design of Novel Mn–C–Al Weight-Reduced Steels

*H. Springer, J.B. Seol, I. Gutierrez, D. Raabe*

Department of Microstructure Physics and Alloy Design

A novel class of steels containing high amounts of manganese (Mn), aluminium (Al) and carbon (C) – also referred to as 'Triplex' steels – offers a low mass density, improved corrosion resistance, high strength and excellent ductility in comparison to conventional steels for structural engineering applications. Profound changes of their mechanical properties can be achieved via aging of the material. More specific, κ–Al(Fe,Mn)$_3$C carbides were found to precipitate from the mainly austenitic matrix, growing from C-enriched areas most probably formed via spinodal decomposition during quenching [1,2]. Further development of high strength Mn–C–Al weight reduced steels necessarily involves the investigation and understanding of both fundamental phenomena as well as more application related parameters. The use of high-throughput bulk combinatorial design methods together with high resolution characterisation techniques applied in a scale-bridging approach enables a rapid maturation of such nano-particle hardened steels. First observations revealed that some of the observed hardening phenomena were highly composition dependent. Determining the optimum material composition and microstructural state by use of conventional metallurgical synthesis and processing methods, however, is often too time-consuming for probing a wider range of chemical compositions each combined with a large matrix of thermo-mechanical routes. For this reason a systematic but accelerated screening of different compositions and heat treatment variants of such steels was introduced.

The novel bulk rapid alloy prototyping (RAP) approach [3] enables for the first time a systematic and simultaneous evaluation of the compositional and thermomechanical trends associated with the change in the Al content for a group of 30Mn–1.2C (wt.%) Triplex steels. Five alloy compositions each exposed to nine different heat treatments were synthesized, processed and evaluated within 35 hours. The mechanical properties of these 45 different material conditions are shown in Fig. 1 in terms of the yield strength (a), ultimate tensile strength (b), total elongation under tensile load (c), and indentation hardness (d). Pronounced trends in the mechanical behaviour of the materials can be clearly distinguished, associated with the changes in chemical composition and aging parameters: Without the addition of Al the most favourable mechanical properties are obtained for the as-homogenised state. As with Mn–C TWIP steels exhibiting similar properties, the embrittlement during aging can be related to the formation of coarse pearlitic particles on the grain boundaries [4]. High amounts of Al (~8 wt.%), on the other hand, show pronounced strengthening during aging, related to the formation and growth of κ carbides. Alloys with intermediate Al concentrations (about 2 to 6 wt.%) do not reveal mechanical properties on the same level compared to the aforementioned extreme cases in their respective optimal conditions. On the other hand, a much

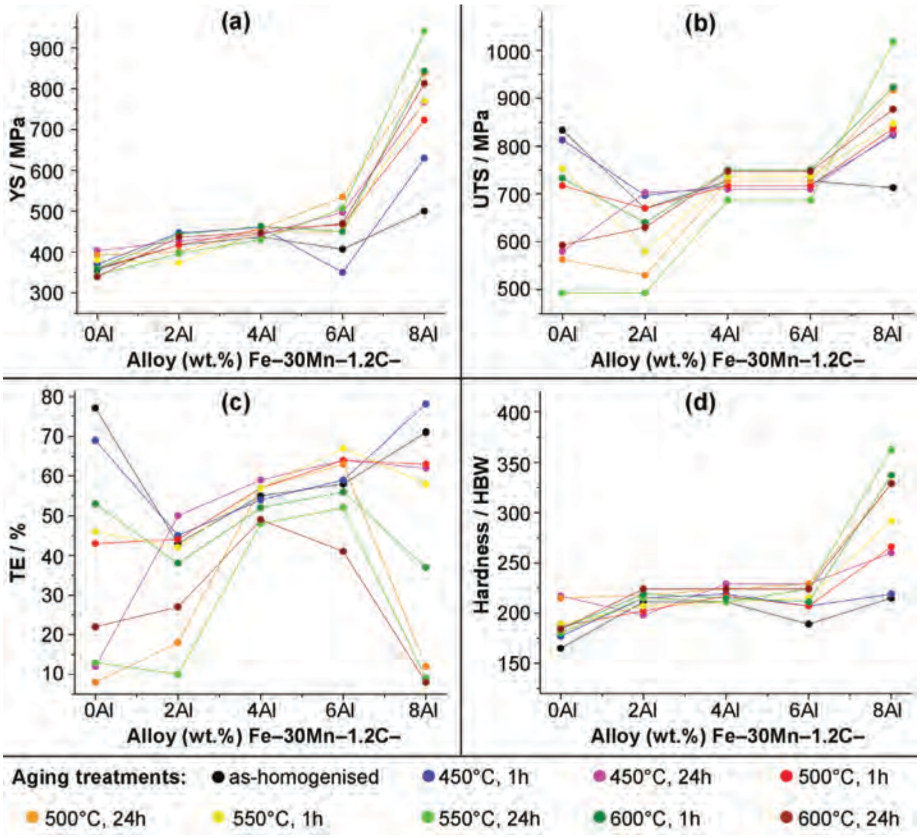

**Fig. 1:** *Overview of the mechanical properties of 30Mn–1.2C (wt.%) based steels obtained by high throughput bulk combinatorial screening as a function of Al concentration and applied ageing treatment: (a) Yield stress (YS), (b) ultimate tensile stress (UTS), (c) total elongation (TE), (d) hardness.*

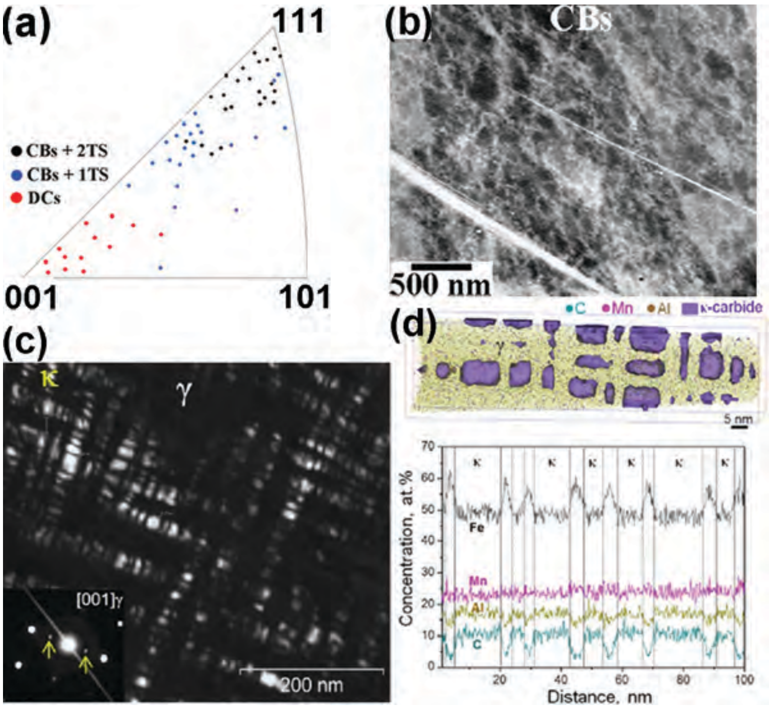

**Fig. 2:** *High resolution characterisation of a 30Mn–1.2C–2Al (wt.%) steel: (a) Crystallographic orientation dependence of the deformation microstructure; CB: cell blocks, TS twinning system, DC: dislocation cells, (b) ECCI image of CBs, (c) DF-TEM image of nano-sized carbides, (d) 3D-APT reconstructed volume and 1D composition profile of κ carbides.*

smaller influence of the aging parameters on the tensile behaviour can be observed in these cases.

The corresponding understanding of the underlying strain hardening mechanisms of Fe–Mn–Al–C alloys requires investigating the microstructure using high resolution characterisation techniques (Fig. 2). The application of the recently developed SEM/EBSD-based ECCI set-up [5] to the characterisation of deformation structures of high-Mn lightweight steels has brought new insights into the respective strain hardening mechanisms [6,7]. Fig. 2(a) shows the grain orientation dependence of the deformation structure in a Fe–30Mn–1.2C–2Al (wt.%) steel, tensile-deformed to 0.3 true strain with a strength of 1.15 GPa. Three types of grains can be systematically distinguished: The first group of grains are characterized by a dislocation cell structure with low deformation twinning activity. These grains occupy an area fraction of about 10 % and are oriented close to <001>//TA (tensile axis) within an angular range of about 15° (red dots in Fig. 2(a)). The average cell size in these grains is 180 ± 40 nm and their shapes depend on the number of slip systems activated. The second group represents grains that contain combined dislocation and twin substructures formed by dislocation cell blocks and lamellar twin structures. They reach about 30 area% and have <112>//TA orientation (±15°; blue dots in Fig. 2(a)). The third group contains grains which build up complex substructures consisting of dislocation cell blocks and multiple-twin substructures. These grains, which are oriented close to <111>//TA with about 15° scatter (black dots in Fig. 2(a)), are the most frequent grains with about 60 area %. At 0.3 true strain, the average cell block size in <111> and <112> oriented grains is 220 ± 50 nm, Fig. 2(b).

Additional nano-structural investigations via TEM and APT give insight into the structural and chemical interactions between matrix and precipitated κ-carbides within Mn–C–Al light weight steels. Fig. 2(c) shows a dark field TEM micrograph and the corresponding selected area diffraction (SAD) pattern of an Fe–30Mn–1.2C–8Al (wt. %) alloy after aging of 600 ºC for 24 h followed by tensile deformation to 15 %. The resultant microstructure is composed of an austenitic matrix containing κ-carbides of cuboidal shape (size ~20 × 10 nm) surrounded by micro- and nano-channels. SAD of the [001]γ zone axis confirmed that the κ-carbides have a cube-cube orientation relationship with the matrix, namely [100]γ//[100]κ, similar to that of γ/γ' interfaces in nickel-base superalloys. Clear {100} superlattice reflections of the κ-phase are caused by an ordering process of interstitial C at the body centered site of the κ-phase with an L'$1_2$ type crystal structure. Fig. 2(d) displays a reconstructed APT map of C (blue) for the aging treated sample and the corresponding iso-surface (purple) of 0.9 at.% C. Both the C-enriched features and the nano-channels as shown in the TEM image in Fig. 2(c) can be detected in the APT data. Using 1-D composition profiles, the partitioning of solutes to different phases can be quantified in terms of an enrichment factor, ε = (at.% in κ-phase) / (at.% in austenite). The ε value for Mn is substantially lower than for Al and C. It seems that Mn atoms are energetically stable inside either the intermetallic κ or austenite phase. This means that the partitioning of solutes to κ-carbides can be controlled by the abutting phase [8]. APT results suggest that during the decomposition of austenite into κ, both matrix (austenite) and product phase (κ-carbide) compete for Mn.

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# Nano-Diffusion Controls Macro-Deformation of High Strength Steels

*S. Sandlöbes* [1], *T. Hickel* [2], *A. Dick* [2], *I. Bleskov* [2], *J. Neugebauer* [2], *D. Raabe* [1]

[1] Department of Microstructure Physics and Alloy Design
[2] Department of Computational Materials Design

Advanced structural materials can have extraordinary mechanical properties due to the interplay of deformation processes on different length scales. During a transformation induced plasticity (TRIP) the atomic structure adapts to an external strain by performing a martensitic phase transformation. Alternatively, materials showing twinning induced plasticity (TWIP) make use of twin boundary formation. In both cases the material responds to plastic deformation by locally adapting the sequence of atomic layers in the region affected. This is only possible, if the stacking fault energies (SFE) are sufficiently low. Changing the chemical composition of a material is the most suitable strategy for adjusting the SFE and in this way purposely designing materials with tailored mechanical properties. Particularly promising are austenitic steels, in which the face-centred cubic (fcc) crystal structure is stabilized by Mn [1].

Carbon is another element with a high relevance for deformation mechanisms in steels. However, the available experimental investigations on the dependence of the SFE on the carbon content seem to be inconsistent: Previously published transmission electron microscopy (TEM) experiments show only a very slight change of the SFE with the C content in steels [2], whereas XRD experiments suggest a strong increase of the SFE in austenitic steels [3] (Fig. 1). Within this article we argue that this discrepancy is due to nano-diffusion processes (diffusion over a few neighbouring sites) in the vicinity of the stacking fault – a result, which was only achievable by combining an in-depth theoretical understanding with new ideas for *in situ* TEM experiments.

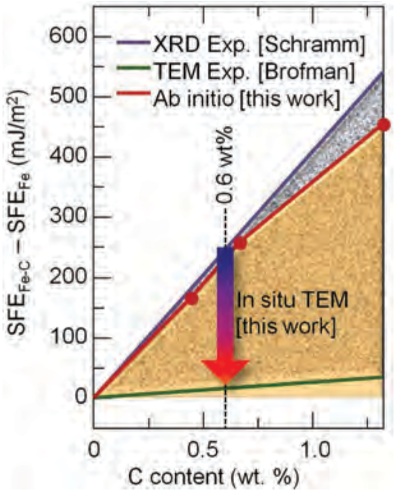

**Fig. 1:** *Dependence of the stacking fault energy (SFE) in steels on the C content. The experimental range of values (textured area) is constraint by XRD experiments (blue line, [3]) and TEM experiments (green line, [2]). Our ab initio results for the Fe-C system yield at T = 0 K a strong increase of the SFE with C content (red line), but imply a reduction of the SFE with increasing temperature (orange area). The arrow indicates the concentration for which in situ (temperature dependent) TEM experiments have been performed in this work. Within the displayed range a reduction of the SFE by 30-40 % has been directly observed.*

*Ab initio* methods are considered to be particularly suitable if accurate chemical trends for structural quantities like the SFE are needed [4]. We have therefore investigated the role of interstitial carbon, performing both supercell calculations that explicitly contain stacking faults as well as bulk calculations used as input for an approximate (ANNNI = Axial Next-Nearest Neighbour Ising) model [5]. A large number of concentrations and configurations of C atoms has been considered. All these calculations are remarkably consistent with each other and in particular with those experiments that show an enormous increase of the SFE with the carbon content (Fig. 1).

The *ab initio* calculations shown in Fig. 1 are performed for a homogenous C distribution throughout the sample, i.e., ignore possible changes of the local chemistry due to the formation of the stacking fault (Fig. 2a). This assumption is well justified in the undeformed state and will prevail after the formation of stacking faults, if C remains trapped in the octahedral sites and is dragged with the lattice during the diffusionless rearrangement of the metal atoms. This is a realistic scenario at room temperature, since at these temperatures the diffusion of C in fcc Fe is known to be negligible. To estimate the local gradients in the carbon chemical potential induced by forming an intrinsic stacking fault (ISF) we have performed supercell calculations that contain such a

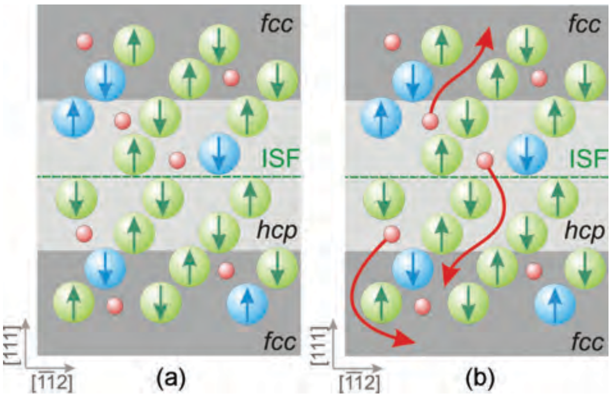

**Fig. 2:** *Two scenarios for the distribution of C in the vicinity of an intrinsic stacking fault (ISF). (a): C is homogeneously distributed, (b): nano-diffusion of C out of the hcp region occurs.*

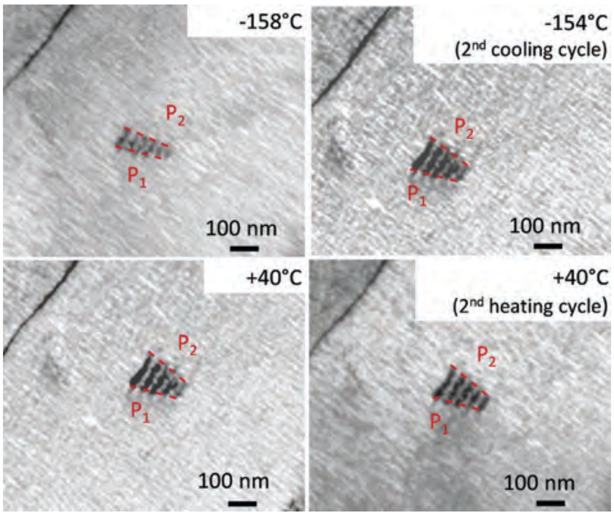

**Fig. 3:** *Change of the dissociation width in Fe-22Mn-0.6C during in-situ cooling and heating in the TEM. The oscillation contrast of the stacking fault of the pre-deformed sample (0.5 % eng. strain) was obtained under adjusted diffraction conditions. During the first cooling-heating cycle (left micrographs) the dissociation width of the partial dislocations has increased. A further cooling-heating cycle (right micrographs) did not cause significant changes in the stacking fault width.*

defect. The calculations clearly show that there is a significant thermodynamic driving force to out-diffuse C from the local hcp region that is formed next to an ISF (Fig. 2b). This out-segregation of solute elements away from the defect is opposite to the conventional well-known Suzuki effect. We therefore termed it anti-Suzuki effect. This effect sets in when the C atoms become mobile, i.e., at sufficiently high temperatures. The C depleted SF-region, as a consequence, has an energy similar to a steel with low/zero C content.

The above described mechanisms become crucial when probing such a situation by electron optical methods: The irradiation of solids by an electron beam via TEM induces scattering events, which can result in an energy exchange between electrons and matter. The influence on possible temperature-activated mechanisms due to the interaction with the electron beam is, however, typically not taken into account when measuring SFEs. We argue that depending on the TEM set-up and the investigated steel these scattering events can locally yield diffusion of C during the measurement, allowing them to follow the strong thermodynamic driving force identified by the calculations. In contrast, XRD measurements generally do not lead to enhanced diffusion. Together with our *ab initio* data this nicely explains why TEM (where nano-diffusion is expected to be active) and XRD (where it is inactive) show the qualitative differences displayed in Fig. 1.

To verify that the electron beam can have a dramatic effect on C diffusion during observation, we performed *in situ* cooling-heating experiments in the TEM. Before starting the measurement we cooled down the sample using liquid nitrogen in a TEM cooling holder. In this way the mobility of C is in comparison to a room temperature measurement additionally limited, which should reduce the impact of scattering events with the electron beam. Even with this setup the C diffusion cannot be completely suppressed, yielding an uncontrollable reduction of the SFE already at this stage. However, the effect became much more pronounced, when the sample was *in situ* heated to 40 °C during the investigation of a region of interest, i.e. partial dislocations that form a SF, while keeping the same position and orientation. We find in all our *in situ* experiments that the dissociation width of the partial dislocations bounding the stacking fault then increases by about 40-60 % during heating (see Fig. 3). This corresponds to a decrease of the SFE by 30-40 % (lower part of the arrow in Fig. 1) The observation is consistent with the theoretical interpretation: The electron beam activates local C diffusion out of the stacking fault thus enabling the C atoms in the ISF to diffuse to the neighbouring fcc phase during the TEM investigation.

In principle, a large number of further concepts could be used to explain this change of the SFE – all of which have been excluded in additional investigations. A thermodynamic explanation was for example ruled out by *ab initio* based calculations, showing that the pure temperature dependence would yield an increase rather than a decrease of the SFE with heating. Most important is, however, that thermodynamic as well as other concepts would result into a reversible behaviour. In contrast to this, all our *in situ* TEM experiments for which we have performed additional cooling-heating cycles consistently show no significant further change of the SFE after the first cycle (Fig. 3).

We conclude from our combined *ab initio* simulations and *in situ* TEM measurements that a nano-diffusion of C atoms in the region of the stacking fault (anti-Suzuki effect) is responsible for the observed change of the local SFE. Combining DFT calculations and TEM measurements reveals that only the local carbon content plays a decisive role for the local SFE. This result provides direct insight into atomic scale mechanisms that allow one to tailor diffusion and segregation effects by appropriate alloying and thermal treatment, a prerequisite to design microstructures with adaptive deformation mechanisms.

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# Atomic Scale Analysis of the Origin of the Strength of Pearlite

Y.J. Li [1,2], S. Goto [3], C. Borchers [2], P. Choi [1], M. Herbig [1], S. Zaefferer [1], A. Kostka [1],
J. von Pezold [4], A. Nematollahi [4], B. Grabowski [4], J. Neugebauer [4],
R. Kirchheim [1,2], D. Raabe [1]

[1] Department of Microstructure Physics and Alloy Design,
[2] Institute for Materials Physics, Georg-August-University of Göttingen, Germany,
[3] Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Japan,
[4] Department of Computational Materials Design

Pearlitic steel subjected to heavy cold-drawing exhibits tensile strengths above 6 GPa [1] being the strongest structural bulk alloy known. Despite great potential for engineering applications (*e.g.*, suspension bridge cables, tire cords, springs), the correlation between the enormous strength and the microstructure is a matter of debate. The relevant mechanisms include the refinement of lamellar spacing, cementite decomposition, and formation of nanoscaled dislocation substructures. To evaluate these mechanisms it is necessary to precisely assess the concentration change of C atoms in ferrite and cementite upon cold-drawing. We have studied the redistribution of alloying elements and the spacing between phase and subgrain boundaries using atom probe tomography (APT) and transmission electron microscopy (TEM) [2]. In parallel, we have conducted first principles simulations to elucidate the physical origin of the extraordinarily high C concentration in ferrite [3]. This hybrid experimental-theoretical approach is a solid basis for revealing the origin of the strength of pearlite.

Our experimental results clearly show that the C concentration in cementite decreases with decreasing thickness of the cementite lamellae (Fig. 1a). This indicates the important role of dislocation drag in the decomposition of cementite which can be explained by an increasing interface-to-volume ratio [2]. Our first principles calculations support this statement. Fig. 1b shows that thermodynamics alone cannot account for the high C concentration in ferrite, leaving the dislocation drag as the most probable solution [3]. First theoretical results for dislocation drag are shown in Fig. 2. In particular, we present the potential energy surface of a C atom around a dislocation. This type of energy surface is a powerful tool allowing to investigate the preferential sites and diffusion barriers of an interstitial atom (here C interstitial) in a host matrix (here Fe). Fig. 2 shows that in the dislocation core region an energy 'tunnel' opens (indicated by the arrow) which corresponds to a lower energy level than in the bulk. This means that C atoms are more stable in the core region and can thus be trapped by a moving dislocation. This is a possible explanation for dislocation drag and thus, in general, our results support C enrichment of ferrite by dislocation drag.

Another important question we could recently clarify is: what generates high strengths at strains >3.5? Increasing strength at strains from 0 to 3.5 is attributed to the refinement of interlamellar spacing

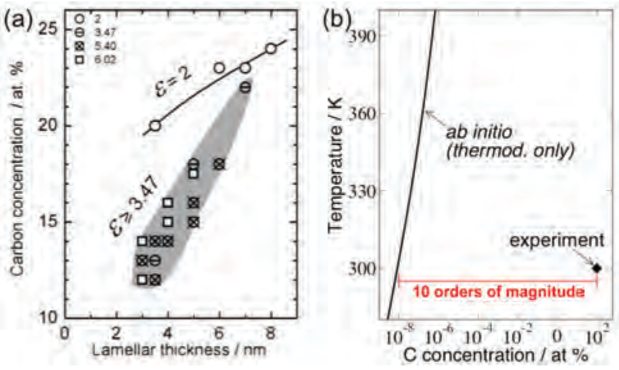

**Fig. 1:** *(a) Experimental C concentration in cementite as a function of the lamellar thickness. (b) Ab initio temperature dependence of C concentration based on a thermodynamic assessment [3], i.e., excluding the drag effect of dislocations. The difference to the experimental concentration is 10 orders of magnitude.*

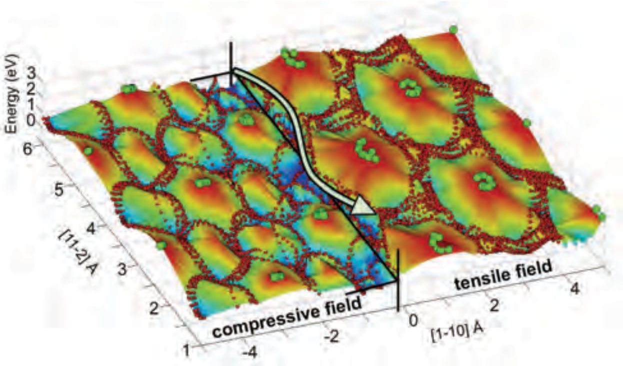

**Fig. 2:** *Energy surface for a C atom diffusing in an edge dislocation in bcc Fe obtained with empirical potentials. The green spheres indicate Fe atoms from several layers projected onto a single plane. The red dots indicate the diffusion paths of a C atom from one interstitial site to the neighbouring.*

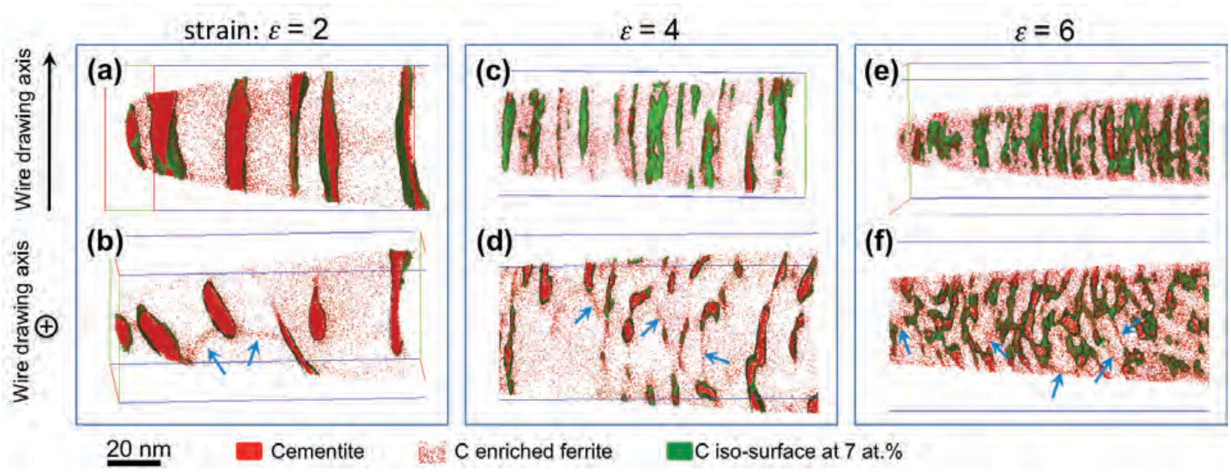

**Fig. 3:** *APT results for true drawing strains 2 (a,b), 4 (c,d), and 6 (e,f) and for longitudinal (a,b,c) and cross-sectional (d,e,f) views of drawn wires. Blue arrows mark some of the (sub)grain boundaries containing excess C.*

and an increasing C concentration in the ferritic regions. At ε > 3.5, however, the C concentration saturates [2], while interfaces gradually lose their strengthening effect due to decomposition and fragmentation of cementite. Fig. 3 shows that in this high strain regime the subgrain size decreases strongly with strain (see blue arrows) providing a possible explanation for the high strength. To support this statement, APT and TEM observations were performed on the ε = 6 wire after annealing which allows a clearer identification. Fig. 4a indeed demonstrates a high density of subgrains. We can exclude that these subgrains were formed during annealing, as low angle grain boundaries are observed (Fig. 4b) which indicates that recovery rather than recrystallization takes place during annealing, since primary recrystallization would lead to high-angle grain boundaries. The observation also indicates that the dislocation substructures have already been formed during cold drawing and that they contribute to the strength of pearlite at ε > 3.5.

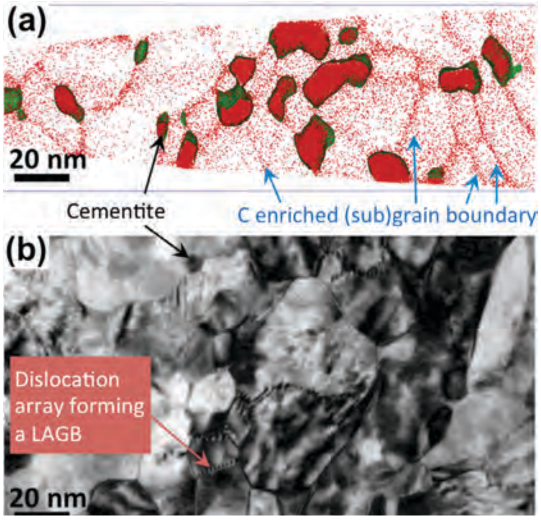

**Fig. 4:** *Nanoscaled dislocation substructures characterized by (a) APT and (b) TEM (bright-field) in the transverse cross-section of a cold-drawn (ε = 6) hypereutectoid pearlitic wire after annealing at 350°C for 0.5h. The green-colored iso-concentration surfaces for 7 at.% C show spheroidization of the originally lamellar cementite during annealing. A dislocation array forming a low-angle grain boundary (LAGB) is marked.*

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# Phase Formation, Phase Stability and Evolution of the Microstructure in Al-rich Ti−Al

*M. Palm*[1]*, N. Engberding*[1]*, F. Stein*[1]*, K. Kelm*[2]*, S. Irsen*[3]

[1] Department of Microstructure Physics and Alloy Design / Department of Structure and Nano-/Micromechanics of Materials
[2] German Aerospace Center (DLR), Cologne, Germany
[3] Research center caesar, Bonn, Germany

Ti−Al based alloys comprise a new class of light-weight alloys with outstanding high specific strength, which enables application up to about 800 °C. Alloys are successfully used for the production of exhaust valves, turbo charger rotors and compressor blades. Though consisting out of two inherently brittle intermetallic phases, TiAl + $Ti_3Al$ lamellar microstructures have been designed, which yield sufficient ductility combined with high strength. Because oxidation resistance at high temperatures is still insufficient, Al-rich TiAl alloys have come into focus recently. It has been shown that also in these alloys lamellar TiAl + r-$TiAl_2$ microstructures can be generated [1] by which mechanical properties may improve [2]. However, lacking knowledge about phase formation and phase stability in the Al-rich part of the Ti−Al system hampered any aimed alloy development.

In order to clarify phase formation and stability in the Al-rich part of the Ti−Al system, a couple of Ti-60 at.% Al alloys have been produced by different techniques to generate different initial microstructures. Kinetics were studied by annealing for varying times and different temperatures. Quenched microstructures were analysed by light-optical, scanning electron (SEM), and transmission electron microscopy (TEM) and *in situ* heating and cooling experiments through differential thermal analysis (DTA) and TEM have been performed to verify results obtained on the quenched samples [3].

In Al-rich TiAl, which becomes supersaturated in Al during cooling, two metastable phases, $Ti_3Al_5$ and h-$TiAl_2$, form (Fig. 1) [4]. $Ti_3Al_5$ forms instantly on cooling while h-$TiAl_2$ is not present in all as-processed alloys but may only form after a short term anneal, e.g. 900 °C/1 h. That $Ti_3Al_5$ forms ordered domains within TiAl (Fig. 2) [3,5] while h-$TiAl_2$ is always present as a separate phase, explains the more spontaneous formation of $Ti_3Al_5$ [3].

On prolonged annealing below the transformation temperature, the $Ti_3Al_5$ domains coarsen and form a tweed-like $Ti_3Al_5$ + TiAl microstructure [6]. DTA investigations show that the transformation temperature for the dissolution of $Ti_3Al_5$ depends on the prior annealing time, which can be explained by increasing interfacial energies through the development of distinct phase interfaces with increasing annealing time [3].

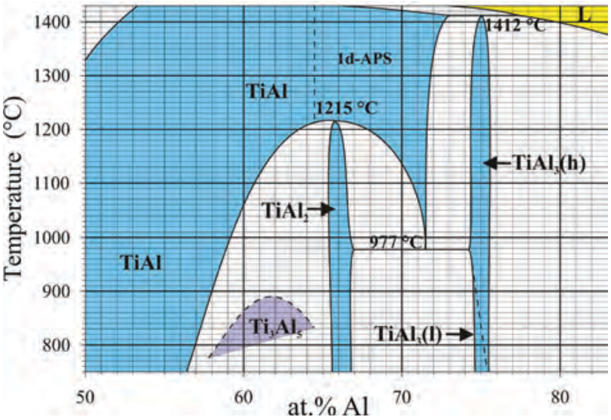

**Fig. 1:** *Al-rich part of the Ti–Al system showing the stability ranges of TiAl, $Ti_3Al_5$ and $TiAl_2$ [4].*

The instant formation of the metastable phases can be explained by a crystallographic analysis. A Bärnighausen tree analysis shows that group-subgroup relations exist between the structures of TiAl and $Ti_3Al_5$ and between TiAl and h-$TiAl_2$, i.e. both transformations are order/disorder transformations, while no such relation does exist for TiAl and r-$TiAl_2$ [7].

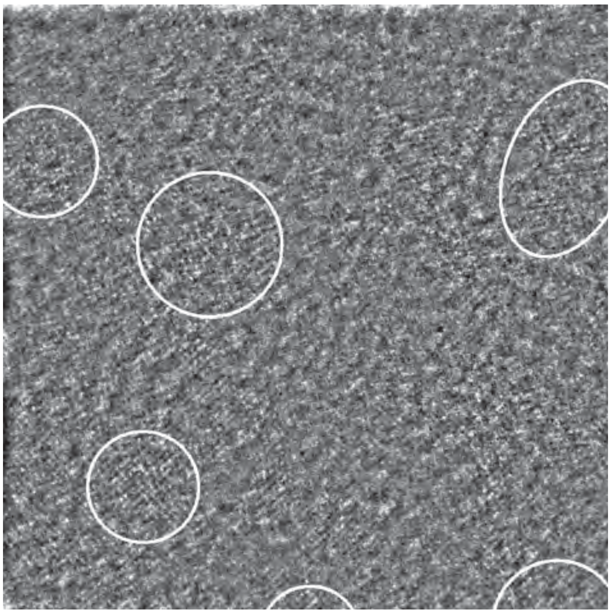

**Fig. 2:** *Fourier filtered high-resolution [001] TEM image (HRTEM) of as-processed Ti-59.7Al showing local $Ti_3Al_5$-type ordering (encircled areas) [3].*

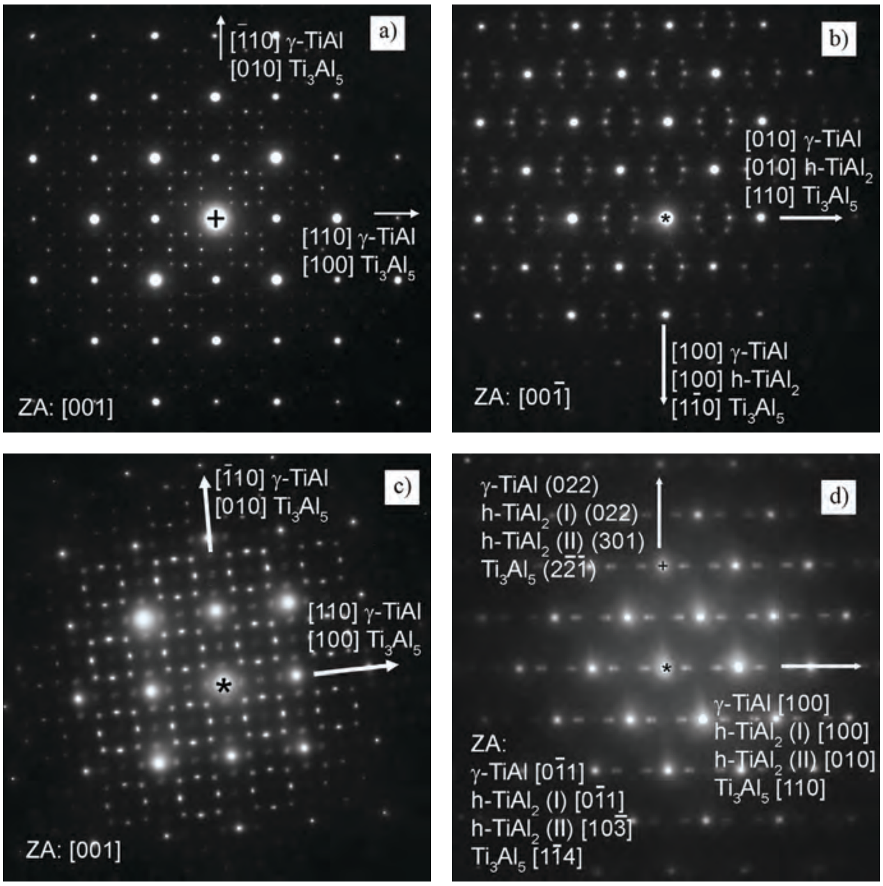

**Fig. 3:** *TEM selected area diffraction (SAED) patterns of differently processed alloys in the as-received condition a) Ti-59.7Al centrifugally cast; b) Ti-59.5Al, c) Ti-60.0Al, and d) Ti-60.5Al levitation melted [3].*

The transformation from metastable h-$TiAl_2$ to r-$TiAl_2$ can happen simultaneously by two different mechanisms, a continuous [8] and a discontinuous one [9], which are characterised by distinct orientation relationships of the resulting r-$TiAl_2$ + TiAl microstructure (Figs. 3-4). The investigation of the kinetics of both reactions reveals that at least at 900 °C the discontinuous reaction proceeds quicker than the continuous one [3].

Also the evolution of the microstructure is crucially affected by the initial microstructure in the as-processed alloys. For an alloy of the same composition and with the same heat treatment a fully lamellar r-$TiAl_2$ + TiAl microstructure can only develop if no h-$TiAl_2$ had been present at grain boundaries in the as-processed alloy because supersaturation with Al is apparently a prerequisite for the formation of a fully lamellar r-$TiAl_2$ + TiAl microstructure [3].

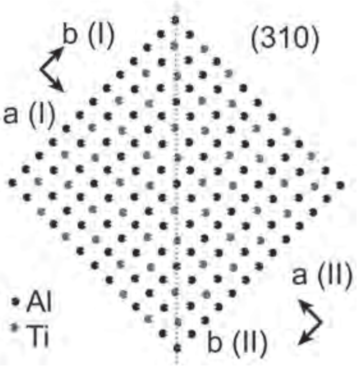

**Fig. 4:** *Illustration of a $\{310\}_{h\text{-}TiAl2\ (I)}//\{310\}_{h\text{-}TiAl2\ (II)}$ rotational twin boundary between the two differently oriented types of h-$TiAl_2$. A projection of a slab with a thickness of six unit cells on the (001) plane is shown [3].*

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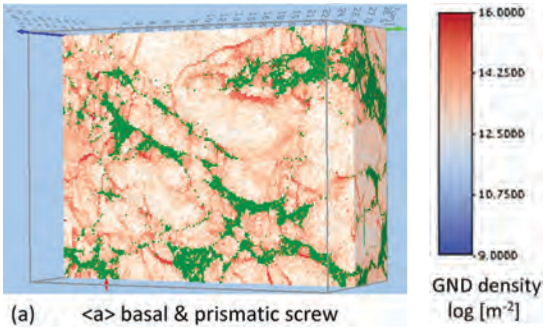
# Design of Ductile Mg Alloys Based on Combined *Ab Initio* and Experimental Methods

*S. Sandlöbes [1], M. Friák [2], Z. Pei [2], L. Zhu [2], F. Wang [1], J. Chen [1], S. Zaefferer [1], J. Neugebauer [2], D. Raabe [1]*

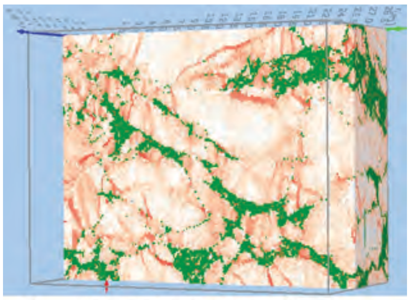
[1] Department of Microstructure Physics and Alloy Design
[2] Department of Computational Materials Design

Magnesium based alloys are attractive for many engineering structural applications owing to their low mass density and high specific strength. However, wide industrial application of Mg is limited by its poor room temperature formability, which is caused by pronounced basal slip and a strong basal texture. Hence, the von Mises criterion requiring five independent deformation modes is not fulfilled. In hcp crystals deformation along the crystal c-axis can only be accommodated by the activation of non-basal slip and deformation twinning. Single-phase solid-solution Mg−Y alloys show an increase in room-temperature ductility by about 5 times compared to conventional Mg alloys, while maintaining a comparable strength and well balanced work hardening. Using 3-D EBSD (Electron Backscatter Diffraction) orientation microscopy to calculate the density of geometrically necessary dislocations (Fig. 1) and transmission electron microscopy (TEM) [1] we show that this ductility increase is related to higher activities of <c+a> dislocation slip providing a <c>-deformation component in Mg−Y.

We show by joint TEM measurements and *ab initio* calculations that this enhanced 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 (SFE) [3]. Both approaches show that the $I_1$ SFE is decreasing with increasing Y concentration (Fig. 2). The reduction of the $I_1$ SFE can be used to explain the ductility increase in the Mg−Y system: 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 stacking fault $I_1$ ($SFI_1$): the sessile $SFI_1$, whose energy decreases with Y alloying, is bound by pyramidal partial dislocation. This enables the formation of dislocation structures on pyramidal planes.

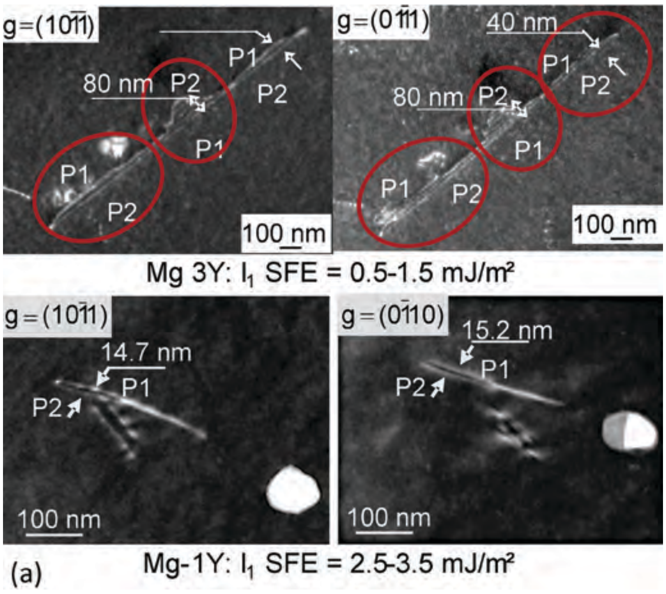


(a) <a> basal & prismatic screw



(b) <c+a> pyramidal screw & edge

**Fig. 1:** *3D EBSD-based orientation microscopy on 30 % cold rolled Mg−3Y (wt.%) displaying the local density of geometrically necessary dislocations (GND) calculated using the Nye tensor approach. Green areas indicate deformation bands [2].*



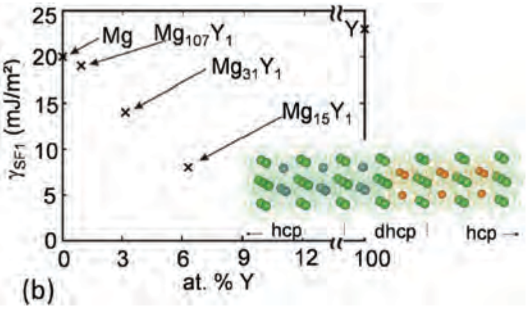


**Fig. 2:** *(a) TEM micrographs showing the $SFI_1$ in Mg−3Y and Mg−1Y (wt.%) for the different diffraction vectors g; P1 and P2 are the bounding partial dislocations, respectively. (b) Ab initio calculated $SFI_1$ energies of Mg−Y alloys [3].*

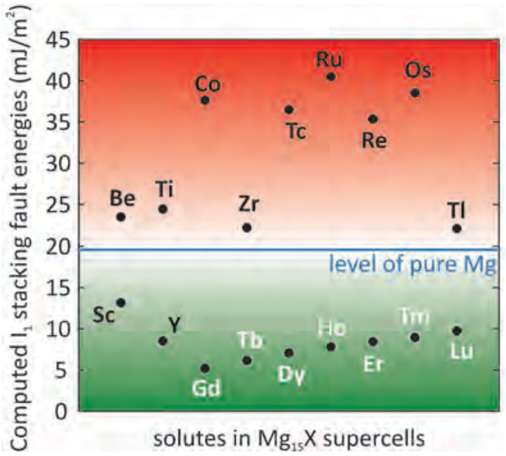


**Fig. 3:** *Theoretically predicted values of $I_1$ SFEs in Mg−X alloys for lanthanides (white) and non-lanthanides (black).*

According to the nucleation model of Yoo et al. [4] we suggest that the SFI$_1$ acts as heterogeneous nucleation source for pyramidal <c+a> dislocations. In summary, the addition of Y causes a reduction of the $I_1$ SFE which leads to the formation of stable SFI$_1$. They provide sources for <c+a> dislocations.

The identification of the $I_1$ SFE as guiding parameter for ductility provides a systematic approach to identify further favourable alloying elements. Following this approach we have performed *ab initio* calculations of the $I_1$ SFE of various Mg−X solid solution alloys (17 in total), Fig. 3. We focused on solutes with hcp structures in elemental state, i.e. matching the crystal phase of Mg [2]. To predict the SFI$_1$ energies, we combined a supercell computational approach with the Axial Next Nearest Neighbor Ising (ANNNI) model [5]. All seven hcp lanthanides reduce the $I_1$ SFE similar to Y (Fig. 3). In contrast, out of 10 non-lanthanide solutes, only Sc alloying reduces the $I_1$ SFE.

Based on these theoretical suggestions we produced five new binary single-phase Mg−X alloys adding elements which were calculated by DFT to decrease the $I_1$ SFE (X; Dy, Tm, Tb, Er, Ho). Tensile testing of the as-homogenized alloys reveals a significant enhancement of the room temperature ductility without a reduction of strength, Fig. 4, nicely verifying the theoretical predictions.

The optical photographs in Fig. 4 show pure Mg and Mg−3Tb (exemplary for all five new alloys) after cold rolling. The observed ductility of the newly designed alloys up to cold-rolling thickness reductions above 40 % reveals the ability of the alloys to accommodate strain along the crystal c-axis. Contrary, pure Mg starts fracturing during cold rolling already after a 10 % thickness reduction along macroscopic shear bands. The EBSD-KAM (Kernel Average Misorientation) maps in Fig. 4 display the local orientation gradients, i.e. strain distribution, in the deformation microstructures. They clearly reveal that the shear bands in pure Mg are resulting from strain localization which is due to an insufficient number of available deformation mechanisms. In contrast, the new Mg alloys exhibit homogeneous strain distribution during deformation. This finding proves the activity of non-basal deformation systems, i.e., non-basal dislocation slip in the new ductile Mg alloys.

In conclusion, we demonstrate that combining *ab initio* calculations with advanced experimental characterization methods facilitates the identification and understanding of critical microstructure parameters as basis for advanced materials design of complex structural engineering materials.

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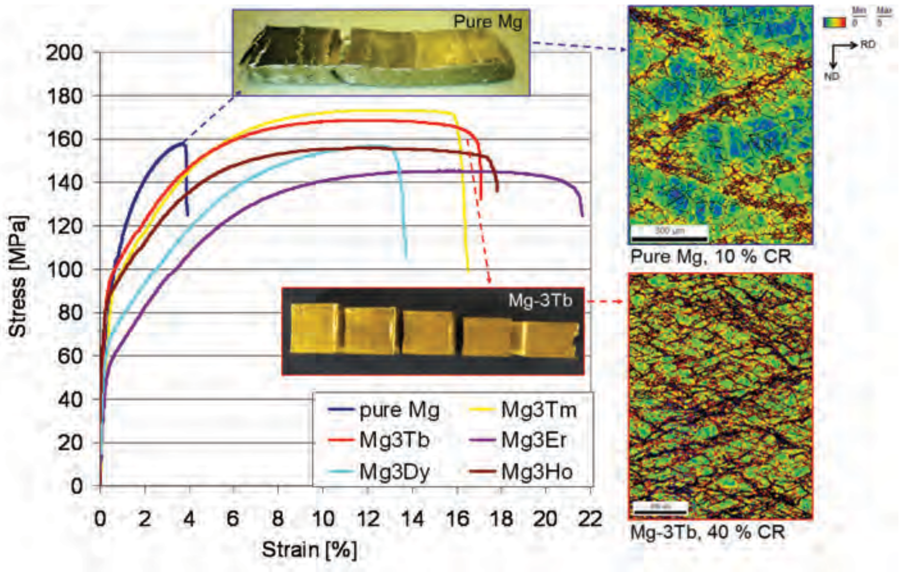

**Fig. 4:** *Tensile stress-strain (engineering strain) curves of the newly designed Mg alloys in as-homogenized conditions in comparison to pure Mg. The optical photographs show the alloys after cold rolling (CR) to different thickness reductions. The EBSD-KAM (Kernel Average Misorientation) maps on the right side display the local orientation gradients, i.e. the strain distribution, from 0° to 5° misorientation.*

# Theoretical-Experimental Investigation of Gum Metal Plasticity

*C. Tasan*[1]*, E. Plancher*[1]*, S. Sandlöbes*[1]*, H. Springer*[1]*, D. Raabe*[1]*,*
*B. Grabowski*[2]*, L. Huang*[2]*, D. Ma*[2]*, M. Friak*[2]*, J. Neugebauer*[2]

[1] Department of Microstructure Physics and Alloy Design
[2] Department of Computational Materials Design

“Gum metal” is a Ti-Nb based alloy developed by a new design strategy that employs *ab initio* simulations to locate vanishing elastic constants resulting in excellent mechanical behavior [1]. The connection between the vanishing elastic constants and the superior mechanical properties is not yet fully understood: while a novel "dislocation-free" and “ideal-bulk-shear” plasticity mechanism had originally been proposed [1], subsequent studies refuted this provocative assumption [2]. The conflict is due to limitations of the employed theoretical and experimental methods. Theoretically, the main shortcoming is the discrepancy with experimental reality: whereas experiments primarily focus on complex compositions (e.g., Ti−Nb−Ta−Zr−O), theoretical approaches are restricted to the simple binary Ti-Nb system [3], with further simplifications due to finite temperature approximations. Experimentally, the variety and complex interplay of the reported mechanisms [2] require to go beyond the typically used post mortem analysis by employing *in situ* investigations.

The new Adaptive Structural Materials (ASM) group (see p. 13) combines on an equal footing state-of-the-art finite temperature *ab initio* expertise and multiscale *in situ* experiments being well suited for these challenges. Our approach to the gum metal problem involves a systematic purification of experimental conditions while improving the theoretical models to overcome the discrepancy between experimental complexity and theoretical simplification. Following this strategy, gum metal compositions with and without oxygen are produced and mechanically tested to verify the critical role of oxygen. To identify the nature of the ideal bulk shear mechanism, samples are *in situ* tested in an as-solution treated condition, since this provides a well-defined microstructure compared to the complex heavily cold-worked marble like structures typically analysed. Following key observations can be drawn from our data: (i) in the absence of oxygen, the specific gum metal properties are lost. (ii) The dominant deformation mechanism is ω transformation-assisted nano-twinning rather than the proposed ideal bulk shear (Fig. 1a-d). Note that the latter conclusion crucially relies on the high-end multi-scale *in situ* experimental techniques available to the ASM group (see also caption of Fig. 1). In future steps, to further

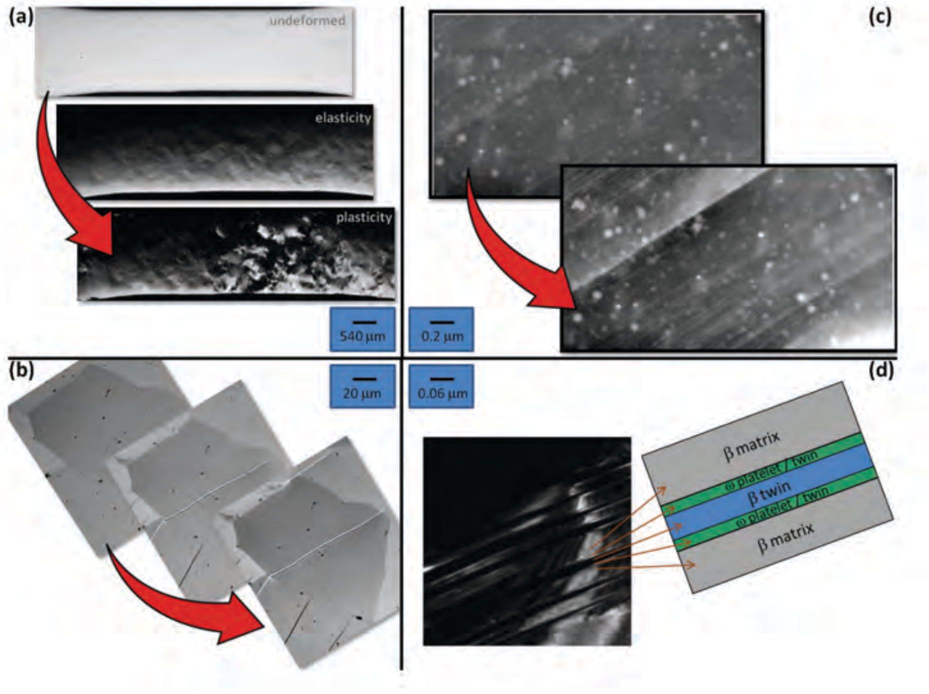

**Fig. 1:** *(a) In situ stereomicroscope testing reveals a significant density of deformation steps on the pre-polished surface. (b) In situ SEM experiments with SE imaging show that these steps, similar to those reported in gum metals earlier [1], have different morphologies than dislocation slip traces or macroscopic twins observed in β-titanium alloys. (c) In situ SEM experiments with BSE imaging reveal that each of the faults has a lamellar morphology consisting of many nano-layers, (d) which are identified in TEM as an internal lamellar-like structure composed of {112}<111> β nano-twins and deformation induced ω phase.*

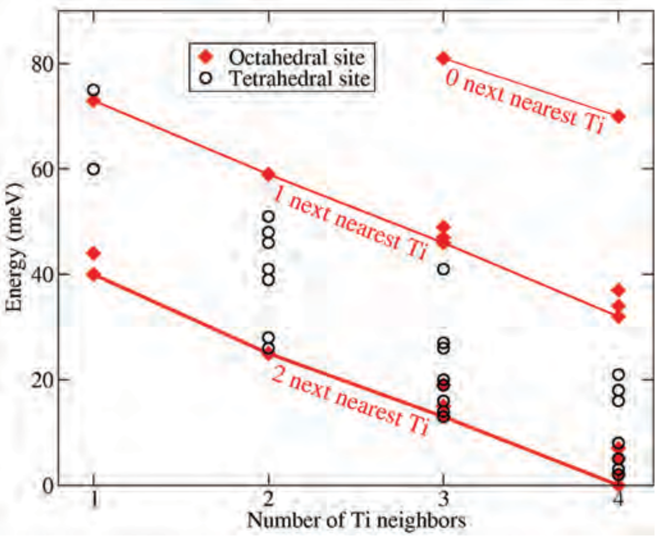

**Fig. 2:** *Ab initio results of the energetics of an oxygen interstitial in Ti-Nb. Energies for a tetrahedral and an octahedral site are shown as a function of the number of Ti neighbors and relative to the most favorable site. For the tetrahedral site, the x-axis refers to the first shell of atoms around the interstitial. For the octahedral site, where the first two shells are needed for an adequate description, the x-axis refers to the second shell while the number of Ti atoms in the first shell is indicated in the figure. The lines are a guide to the eye emphasizing the preference of the O atom to be in a Ti-rich environment.*

increase the connection to theory, simpler Ti−Nb + O ternary alloys of systematically varying composition and thermo-mechanical treatment will be analysed with our *in situ* methods.

Following our experimental findings and additional literature observations [4] regarding the importance of oxygen, the first theoretical steps are directed towards *ab initio* investigations of the energetics of oxygen in Ti−Nb. Fig. 2 shows results for interstitial oxygen in Ti−23 at.%Nb, specifically, for the octahedral and tetrahedral sites as function of the local environment. The relevance of this figure is given by the fact that Ti−Nb is expected to be disordered at finite temperatures and hence the oxygen atom will have different local environments available which can be occupied according to their energies. The simulations reveal three main conclusions: (i) most tetrahedral sites are unstable with respect to the octahedral site. (ii) The O atom prefers a Ti rich environment and (iii) the overall energy scale of the various sites is rather small, suggesting that various sites will be available to the oxygen atom at higher temperatures. Following the strategy noted above, next theoretical steps aim at increasing the theoretical complexity by considering the role of the metastable ω phase and the influence of oxygen on ω stability. A crucial ingredient in this respect is the specific expertise of the ASM group in carrying out accurate *ab initio* simulations at finite temperatures.

In the long term, once the mechanisms and atomistic variables of the gum effect are understood, we plan to use our finite temperature *ab initio* methodology to create maps of instabilities as function of temperature, strain, and composition (Fig. 3), in order to guide the experimental design of new-generation gum alloys with further improved properties.

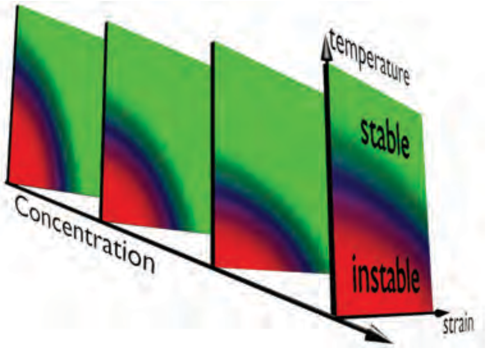

**Fig. 3:** *Schematics of our long-term goal: a 4D representation of an instability map (in terms of elastic constants) as function of different variables (e.g., temperature, strain, and concentration).*

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# Investigations of the Thermal Stability of the Interface Formed during Explosive Cladding of Hastelloy B3 to Stainless Steel

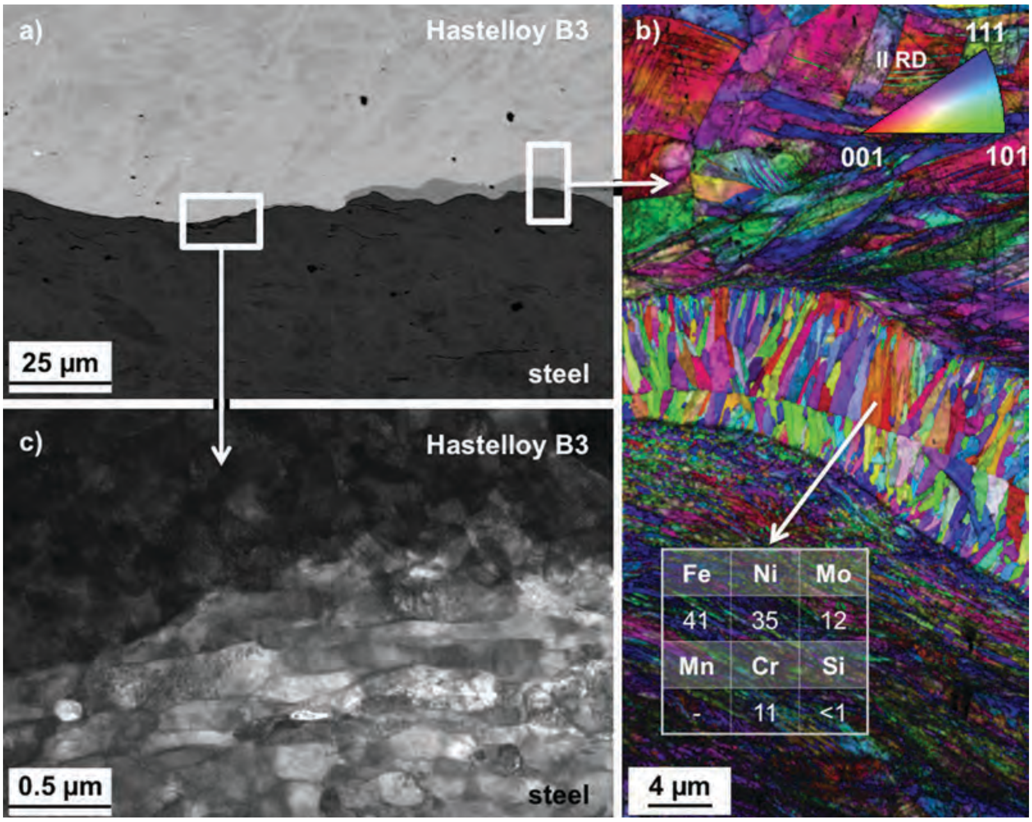
*A. Kostka*[1], *A. Szczepaniak*[2], *D. Raabe*[2]

[1] Max Planck Fellow Research Group on High Temperature Materials
[2] Department of Microstructure Physics and Alloy Design

Metallurgical processes governing microstructure formation in the interface regions of heterogeneous joints are very complex and their understanding requires precise characterization under well defined welding conditions [1]. In this context joints of alloys from the Ni−Mo Hastelloy B family to steel are of high interest from an engineering standpoint owing to their huge relevance in the engineering design of advanced solutions where the combination of high thermal stability and exceptional corrosion resistance is demanded. Alloys from the Hastelloy B family (Ni-base alloy with Mo content up to 32 wt.%) are successfully used for many years, however, they suffer a serious drawback when welding is applied. One of the most important problems is an intergranular brittle fracture mode, where the cracks appear on the surface of the Hastelloy B2 after applied post-welding heat treatment [2]. Thus, a detailed microstructure-oriented understanding and property optimization of the underlying interfaces of the joints between dissimilar bulk metals are essential for the design of modern metallic compounds.

The aim of this investigation is to characterize and better understand the graded microstructures at the bonding zone and their metallurgical formation processes with regard to the mechanical behavior of the cladded joints between Hastelloy B3 (improved thermal stability with respect to the B2 family by optimization residual alloying elements) and austenitic stainless steel [3].

Explosive joining processing leads to (i) intense and localized plastic deformation, (ii) high localized stresses and (iii) high local temperature increase causing both melting and rapid solidification [4]. Fig. 1a shows the microstructure of the interface



| Fe | Ni | Mo |
|---|---|---|
| 41 | 35 | 12 |
| Mn | Cr | Si |
| - | 11 | <1 |

**Fig. 1:** *Analysis of the interface region of the clad: a) SEM (SE) micrograph showing the bond zone and melt pockets; b) inverse pole figure map revealing the microstructure development around the solidified material and its chemical composition (wt.%); c) TEM (BF) micrograph showing direct bonding between joined components (absence of a reaction layer).*

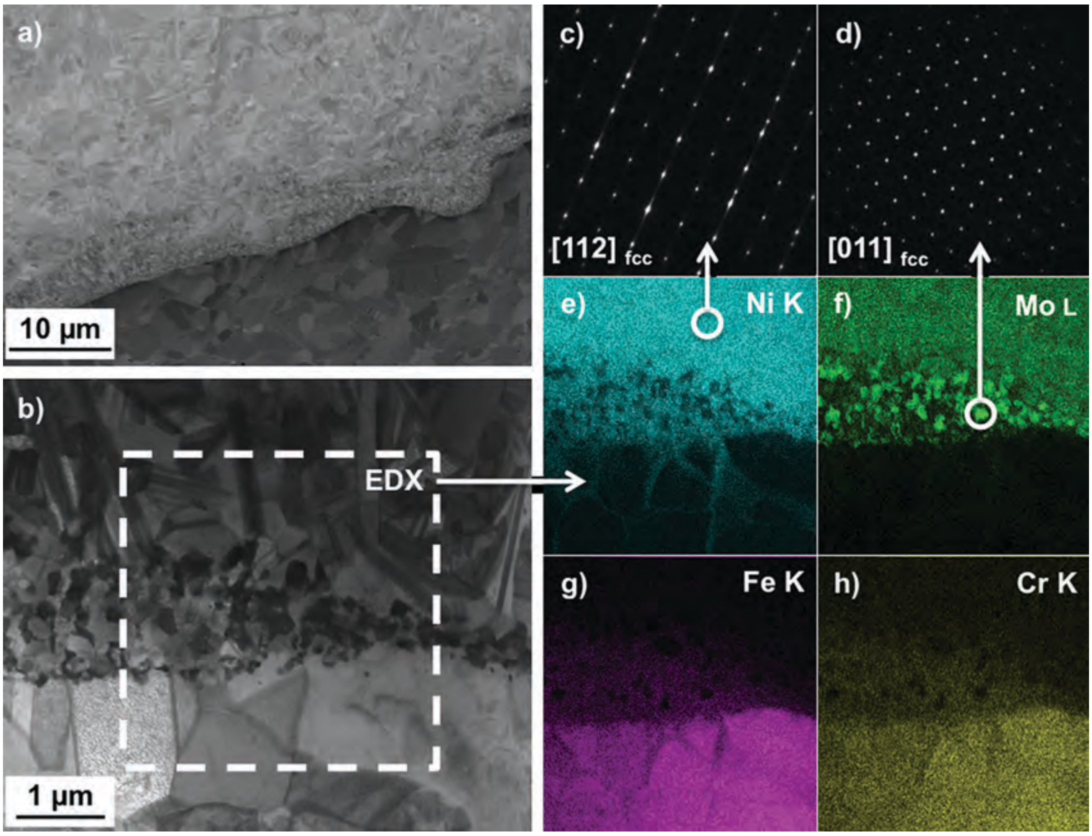


**Fig. 2:** *Evolution of the interface region of the clad after subsequent heat treatment (750°C, 1h, air cooling): a) SEM (SE) micrograph reveals recovery of both parent materials; b) STEM (BF) micrograph reveals presence of twins in the B3 Hastelloy; c) selected area electron diffraction from the B3 Hastelloy and d) precipitated Mo-rich (82 wt.%) phase; e-h) EDX element maps from the highlighted region in b).*

region after cladding. The interface does not reveal a regular wavy morphology (which is otherwise typical of explosive cladding process) but is partially flat. Localized melted regions (Fig. 1b) adjacent to the interface are identified in terms of their characteristic solidification-elongated grain shapes and a strong chemical inhomogeneity resulting from the intense chemical mixing of the joined components. Less than 25% of the interface length consists of melted and solidified regions (measured on the surface parallel to the welding direction at a distance of 1000 µm), thus the dominant type of the interface consists of strongly deformed parent material. TEM examination of this type of interface (Fig. 1c) reveals direct bonding and absence of any reaction products.

The effect of an applied heat treatment (750°C, 1h, air cooling) is presented in Fig. 2. Both parent materials recovered and small Mo-rich precipitates [4] appear at the interface. Acquired EDX maps indicate strong diffusion of Cr from the austenitic steel towards the region of Mo precipitations and Ni from the Hastelloy towards the steel up to 1 µm deep.

The amount of strain accumulated during collision of the joined plates leads to massive coldworking and strain hardening. The applied heat treatment significantly enhances diffusion processes as well as recovery and recrystallization and associated chemical reactions leading to the formation of complex new non-equilibrium phases.

In the following part of the project the correlations between the resulting microstructures and mechanical properties will be investigated in order to identify which of the microstructural constituents formed at the interface region are essential for damage initiation in these complex material compounds.

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# Application of 3-Dimensional EBSD-Based Orientation Microscopy

*S. Zaefferer, P.J. Konijnenberg, D. Raabe*

Department of Microstructure Physics and Alloy Design

3D orientation microscopy based on a combination of electron backscatter diffraction (EBSD) and serial sectioning with a focused ion beam (FIB) offers a number of unique features for microstructure characterization, in particular the full, 5-parameter grain boundary description but also, for example, the description of the 3D morphology of crystals, or the determination of geometrically necessary dislocation (GND) densities. 3D EBSD data sets can be analysed in two approaches, either as volume pixels (voxels) or by reconstructing interfaces and boundaries.

## Voxel-based description of 3D data

After measurement, 3D EBSD data exist first as unconnected voxels. When describing crystalline microstructures it is important to group these voxels into crystallites or subgrains. To this end the measured sections first have to be aligned such that subsequent sections fit together in an optimum manner. Alignment procedures for shifts of complete sections as well as unsystematic misalignments due to drift during the EBSD measurements have been developed.

After slice alignment a segmentation algorithm is used to group voxels into grains. An example for a rendered voxel-based microstructure is displayed in form of an EBSD pattern quality (PQ) map in Fig. 1a for a tensile-deformed low-alloyed TRIP steel. The volume outlined by dashed lines is rendered as an inverse pole figure (IPF) voxel map in Fig.1b for one deformed ferrite grain. A particularly interesting analysis with respect to deformation and phase transformation is the calculation of GND densities according to Nye [1] and Kröner [2]. Fig. 1c displays the total GND density calculated for a fraction of the volume marked in Fig. 1a, in comparison to a 3D KAM (kernel average misorientation) map of the same volume, displayed in Fig. 1d. While the KAM map represents the orientation gradient at every position, the GND map represents, in principle, the curvature of the orientation field.

## 5 parameter grain boundary characterization

3D orientation microscopy can be used to describe the crystallographic nature of interfaces. If one disregards the atomistic level, grain boundaries are comprehensively described by 5 parameters, that is the misorientation across the boundary (3 parameters) and the crystallographic orientation of one of the interface normals (2 parameters) (see, e.g., Rohrer [3]).

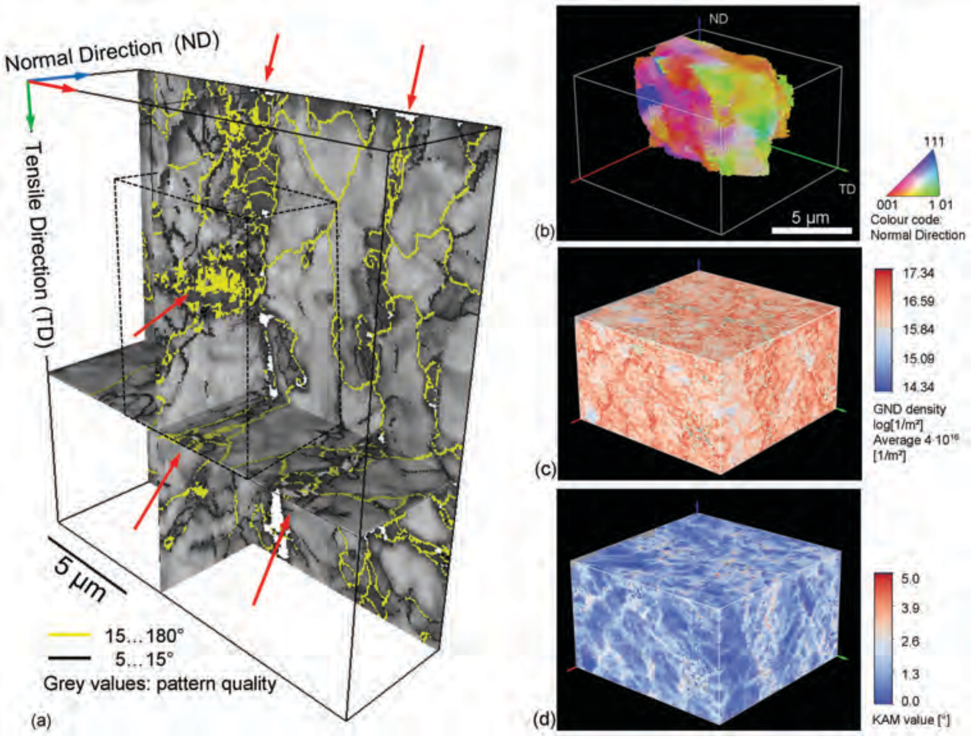

**Fig. 1:** *(a) 3D EBSD pattern quality mapping obtained from a low alloyed TRIP steel deformed in a tensile test almost to fracture (measurement: 60 slices à 100 nm distance). The position of martensite bands is indicated by red arrows. Yellow and black lines indicate large-angle (>15°) and medium-angle (5…15°) grain boundaries. (b)-(d)Voxel-based display of the area marked by dashed lines in fig. (a). (b) Inverse pole figure (IPF) plot of the sheet normal direction (ND) of one grain in the structure. (c) 3D plot of the density of geometrically necessary dislocations (GND) (in log $1/m^2$)). (d) 3D plot of the kernel average misorientation (in degree) calculated for direct neighbours.*

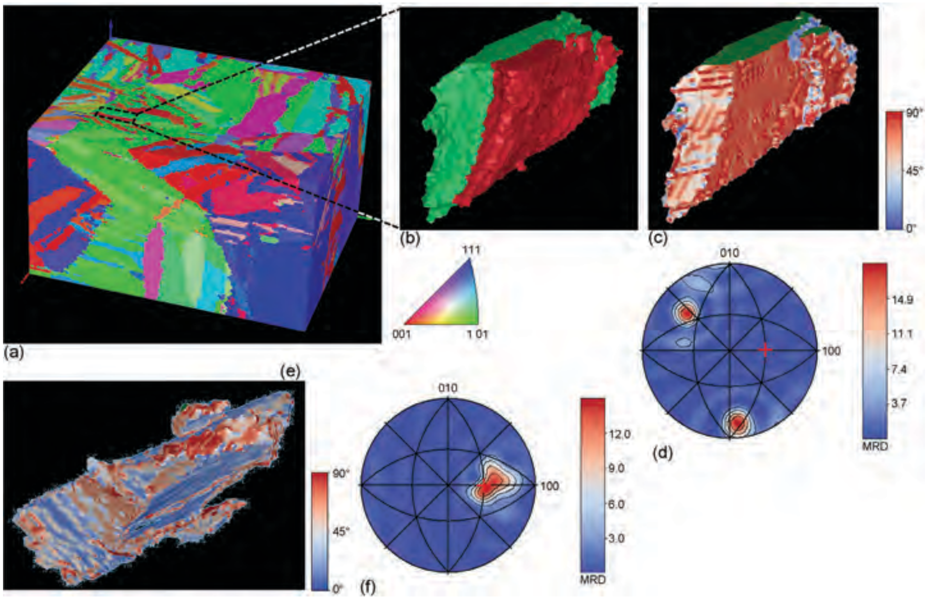

**Fig. 2:** *3D display of the microstructure of an Fe-28% Ni alloy (material supplied by N. Tsuji, Kyoto University). (a) The full block of material displayed as IPF map of the sample normal direction. (b) Two neighbouring plates of lenticular martensite taken from (a). (c) Twist-tilt character plot of the interface between the grains in (b). (d) Grain boundary normal pole figure of the interface from fig. (c) indicating the position of the misorientation rotation axis as red cross. Both grain boundaries have tilt character. (e) Twist-tilt plot of the interface between two other grains. (f) Grain boundary normal pole figure of the grains in (e) indicating a pure twist boundary.*

Boundary reconstruction is composed of two sequential steps; identifying the boundary surface and subsequently translating this surface into a mesh of triangles. A well-known method for boundary reconstruction is the Marching Cubes (MC) algorithm [4] which has been applied for boundary reconstruction from orientation voxels before [5]. The ambiguities inherent to the MC algorithm can be solved by disassembling each cube into unambiguous tetrahedra, resulting in the so-called Marching Tetrahedra (MT) algorithm [6] which has been implemented in our software.

The as-meshed surface structure still requires smoothing because of its inherent roughness and artefacts due to a poor slice alignment. We developed a smoothing strategy [7] which is inspired by computer models for grain growth simulation as implemented in a vertex model by Barrales [8].

In our model, in contrast to classical vertex models, the number of grains must stay constant (thus no topological changes) and quadruple junctions are not allowed to move. All boundaries and triple lines are treated each with a uniform mobility and surface energy. We refer to this approach as a Constrained Vertex Model (CVM) method.

The described algorithms have been employed for the analysis of some selected grain boundaries in a fully martensitic Fe 28% Ni alloy, Fig. 2a. After the grain structure was established the boundary structure was meshed with the MT method and smoothed using the CVM method. In order to describe the grain boundary character three grains were isolated from the microstructure, Figs. 2b and e. The mean disorientation between the grains amounts to about 55°[101] between the grains in Fig. 2b and 53°[323] between the grain in (e) and its (not shown) neighbour. Both grain misorientations correspond to typical disorientations between two Nishiyama-Wassermann variants. The grain boundaries are shown in Figs. 2c and 2e, where the colour code indicates the boundary character in terms of the angle between the disorientation rotation axis and the grain boundary normal. The boundary character is twist if both vectors are parallel and tilt if both vectors are perpendicular. This situation is shown more quantitatively in the pole figures of the boundary normal vectors in Figs. 2d and 2f. The misorientation axis is marked by a cross. Note, that the distinction between twist and tilt boundaries enables an essential geometrical classification of small angle interfaces. Its physical relevance for boundaries with large angle misorientations is, however, limited.

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# Microstructure Effects on Hydrogen Embrittlement in Austenitic Steels: A Multidisciplinary Investigation

*S. Evers[1], T. Hickel[2], M. Koyama[3], R. Nazarov[2], M. Rohwerder[1],*
*J. Neugebauer[2], D. Raabe[3], M. Stratmann[1]*

[1] Department of Interface Chemistry and Surface Science, [2] Department of Computational Materials Design
[3] Department of Microstructure Physics and Alloy Design

Hydrogen atoms, which can be absorbed into steel during production and service, often have a detrimental embrittling effect on the mechanical properties of iron and steels. It is meanwhile known that hydrogen embrittlement (HE) is also affected by the microstructure of the material. Consequently, previous indications that hydrogen atoms are trapped by vacancies, dislocations, and grain boundaries led at MPIE to investigations of superabundant vacancy formation, hydrogen-enhanced local plasticity (HELP), and hydrogen-enhanced decohesion (HEDE). Despite these efforts, any proof of a HE mechanism to be active in a given steel sample has so far been a formidable task, which cannot be achieved by a single method. A direct experimental observation of hydrogen impurities is difficult due to the low solubility and high mobility of hydrogen in steels, whereas pure theoretical investigations are challenged by the complexity and diversity of microstructural features present in steels.

We therefore follow a multidisciplinary strategy to derive a deeper understanding of HE in steels. This strategy combines novel potentiometric methods based on the Kelvin probe technique to detect the local hydrogen content in materials (GO department), *ab initio* determination of the same quantities including the local behaviour at grain boundaries (CM department), and characterization of hydrogen induced materials failure (MA department) using orientation-optimized electron channelling contrast imaging (ECCI). Selected findings of these investigations and their relevance for austenitic steels are summarized in the following:

The crucial idea for the new ***hydrogen detection method*** is the observation that hydrogen dissolved in a palladium matrix leads to the formation of a hydrogen electrode on the palladium surface, even in dry atmospheres. The origin is the presence of a nanoscopic water layer adsorbed on the surface, enabling the formation of a corresponding electrochemical double layer [1, 2]. As the electrode potential for the hydrogen electrode depends logarithmically on the activity of H in Pd, this potentiometric method is extremely sensitive especially at low activities.

The idea can be employed for the investigation of steels (and various other materials) by evaporating a thin film of Pd on their surface. Since the chemical potential of H in iron-based materials is much higher than in Pd, H diffuses into the Pd film. Time dependent measurements of this accumulation can be used to perform extremely sensitive and laterally resolved measurements of H permeation through and its presence in materials. In the latter case an effective “activity” of H is measured, providing information about depth and density of traps sites. Main challenges of this method are the need for an exact calibration of the potential-concentration correlation for H in the evaporated Pd films, the precise calibration of the Kelvin probe tip in the dry nitrogen measurement atmosphere, as well as its long term stability.

As an example the measurement of H in a H-charged austenitic steel sample, comprised of mainly austenitic and ferritic grains, is shown in Fig. 1. It can be seen that the austenite contains much more H, as the potential decreases much faster over the austenite grains. Especially active sites are located at boundaries between ferrite and austenite.

An additional insight into the relevance of the different phases and their boundaries has been

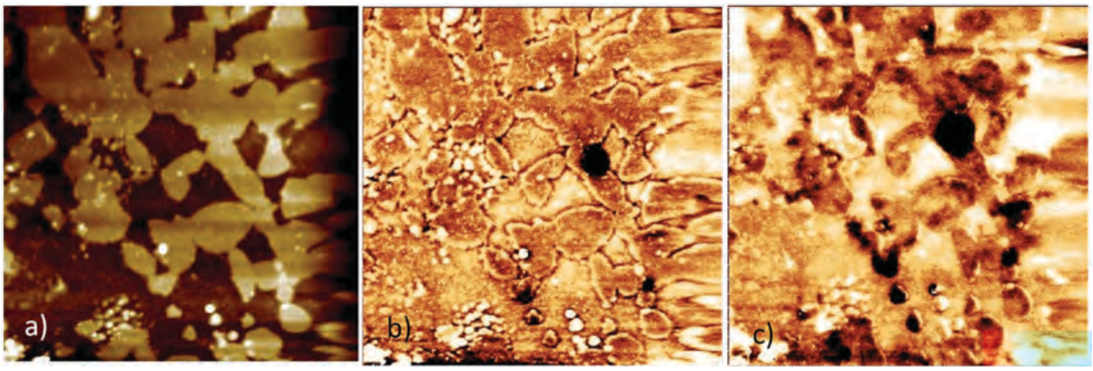

**Fig.1:** *Detecting hydrogen on a $50\times50\ \mu m^2$ surface area of a H charged austenitic steel after evaporation of a 100 nm Pd film. a) A topographic image obtained by AFM indicates austenitic (due to surface preparation topographically higher) and ferritic (lower, i.e., darker) regions. b) and c) Potential maps of this area obtained after 28 h and 44 h in the Kelvin probe mode. Above the austenites the potential decreases faster than above the ferrites due to the larger amount of stored hydrogen. The dark spots in b)-c) indicate sites with especially high hydrogen concentrations (traps).*

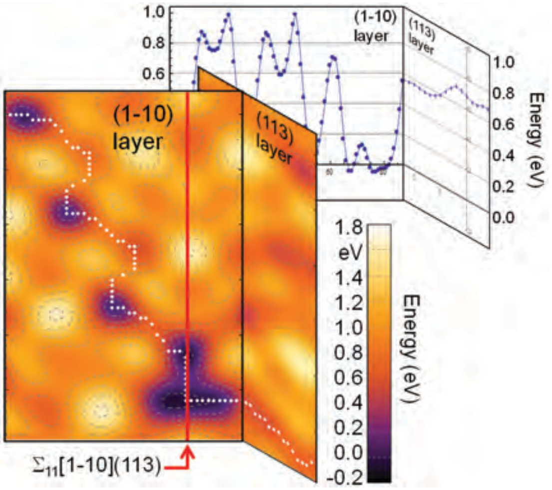

**Fig. 2:** *Potential energy surface for a single H interstitial next to a $\Sigma_{11}$[1-10](113) grain boundary in fcc iron. The minimum energy path for a diffusion in a (1-10) / (113) plane perpendicular / parallel to the boundary is indicated by white dots. In the upper part the corresponding energies along the same path are plotted.*

obtained by ***ab initio calculations*** based on density functional theory (DFT). They clearly confirm the increased solubility of H in austenite grains as compared to the ferrite grains. Mn yields further increase of the austenite solubility by straining the lattice (volume effect). One of the new insights obtained by the calculations is that small amounts of further alloying elements (like Ca, Nb, Si, Ti, and in particular Mo) considerably enhance the preference of H for austenite [3].

In order to understand the experimental results on microstructures, we have additionally used DFT to study the solubility and diffusion of hydrogen in austenite twin and grain boundaries [4]. We generally find that the solution energy of H strongly depends on the local coordination and that it is in this case only moderately correlated with the actual volume of the interstitial site. Within open structures, such as the $\Sigma_{11}$[1-10](113) fcc grain boundary, various different interstitial sites are favorable for the incorporation of H atoms, providing effective trapping centres (Fig. 2). Only if these traps are filled by other H atoms, efficient diffusion channels along (113) planes might become active. We further find that the critical strain required to fracture the material is reduced by the presence of hydrogen in this grain boundary. For twin boundaries, the DFT calculations show that interstitial H atoms are actually slightly repelled. As origin for this unusual and unexpected behaviour the structural similarity between the octahedral interstial configurations in the twins and in austenitic bulk has been identified.

These theoretical insights are highly relevant for experiments, which ***investigate the fracture mode*** in austenitic steels. For this purpose the recently developed orientation-optimized ECCI method has proven to be particularly useful to reveal deformation twins and complex dislocation substructures in TWIP steel. The actual measurements have been performed for a H charged Fe–18Mn–1.2C austenitic steel [5], for which the tensile ductility was drastically reduced by H charging during tensile testing. The central region of these samples, which have not been reached by hydrogen, showed a ductile fracture surface. In contrast, a brittle fracture surface was observed from the surface down to about 150 µm. The facet size of the brittle fracture areas is about 50 µm, which corresponds to the grain size, indicating that intergranular fracture was caused by H charging.

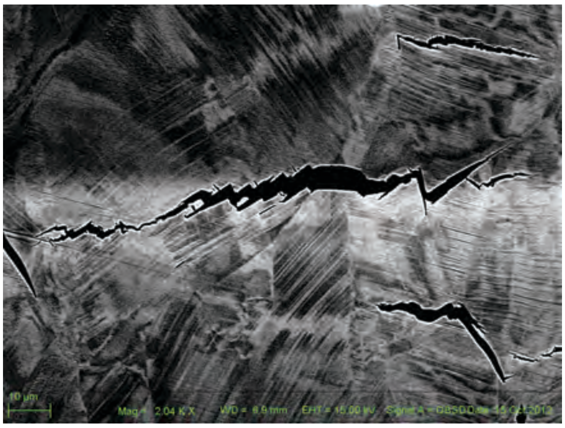

**Fig. 3:** *ECCI micrograph for the crack propagation in Fe–18Mn–1.2C austenitic steel. The cracks initiate at a grain boundary, where deformation twins are intercepting. The crack propagation afterwards continues along the deformation twins.*

An advantage of the employed ECCI method is that in addition to the cracks primary and secondary deformation twins on (11-1) and on (1-11) planes become visible with bright contrast (Fig. 3). The measurements therefore revealed that cracks typically occur at grain boundaries with intercepting primary deformation twins. The stress concentration at these points and the reduction of the cohesive energy by hydrogen loading apparently yields crack initiation. While the primary fracture mode is intergranular, one additionally observes crack propagation following primary and secondary deformation twin boundaries (Fig. 3). Since the *ab initio* calculations predict that perfect twin boundaries are not sensitive to H, the stresses due to the interception of twins with grain boundaries or of primary with secondary twins need to be responsible for such a transgranular fracture along twin boundaries. Being crucially important, because deformation twinning is essentially required to achieve the superior mechanical properties of TWIP steels, further investigations of this effect are currently performed.

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# Absence of an Intrinsic Mobility for Grain Boundary Migration

*C.P. Race, J. von Pezold, J. Neugebauer*

Department of Computational Materials Design

The migration of grain boundaries in polycrystalline materials plays a crucial role in the evolution of microstructure in processing and application. A clear picture of how grain boundaries move is necessary for a full understanding of the mechanical properties of materials and will help enable the design of new materials to meet current technological challenges.

Direct simulation of the evolution of the grain boundaries in a polycrystal under realistic conditions lies beyond the timescales achievable with atomistic simulation techniques such as classical molecular dynamics (MD). MD is thus frequently used rather as a tool to explore fundamental properties of isolated grain boundaries in bicrystals. These properties can then form inputs to larger length and time scale models.

This reductive approach gives rise to the concept of an "intrinsic mobility" of a grain boundary of a given geometry: a constant of proportionality between the velocity with which the boundary moves and the thermodynamic driving force for its motion. MD simulations (and experiments) in bicrystals might then be used to map out these intrinsic mobilities as functions of grain boundary structure.

The study of grain boundary migration with MD is still in its infancy and many mysteries remain to be solved. In particular, little is known in detail about grain boundary migration mechanisms. We have therefore undertaken extensive investigations of a model boundary – the [111] $\Sigma 7$ symmetric tilt boundary – in order to understand its migration mechanism and how this affects the measured mobility.

We have focused in particular on the smooth (i.e. at temperatures below the roughening transition) flat (i.e. curvature-free) boundaries frequently used as a basis for measuring intrinsic mobility in simulations and experiment. By extending our analysis to larger system sizes and smaller driving forces than those typically used, we find that key assumptions about the migration kinetics do not hold. The boundary velocity $v$ is not proportional to the driving force (Fig. 1a) and instead shows a finite threshold force for migration and an upward curvature. An Arrhenius plot of $\ln(v)$ against inverse temperature ($1/T$) (Fig. 1b) reveals that there is no single activation energy barrier for grain boundary migration: the barrier depends both on the driving force and on the temperature. We find that the grain boundary velocity depends strongly on the system size (Fig. 1c).

As the origin of this unexpected behaviour, we have identified that at the mesoscale the migration mechanism involves the formation and growth of islands of crystal volume transformed from the thermodynamically disfavoured to the favoured orientation (Fig 2a). Thus the migration of smooth flat boundaries involves a homogeneous nucleation process: for migration to take place an island of migrated material must form of sufficient radius $r$ that the free energy cost of creating the edge of the island is compensated by the free energy gain of the island volume in the more stable orientation. The need to stabilise a critical nucleus naturally explains the threshold driving force for motion evident in Fig. 1a. As the driving force for migration is increased,

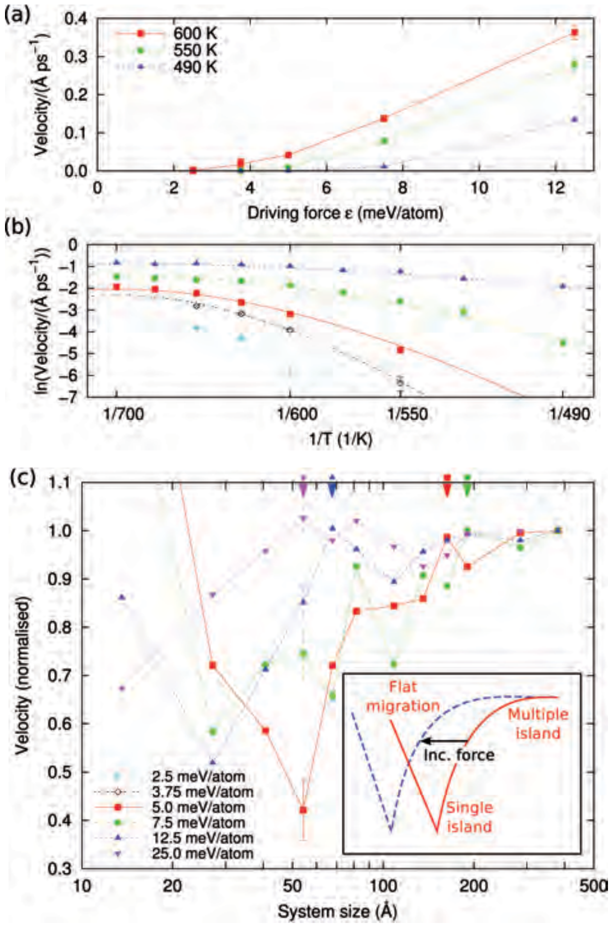

**Fig. 1:** *Results of MD simulations of our grain boundary. (a) The velocity as a function of driving force at several temperatures.(b) An Arrhenius plot of the velocity as a function of temperature for several driving forces (symbols are as for the key in figure (c)). The lines are predictions of the island free energy model. (c) The normalised velocity at 600 K as a function of system size (cell dimension in grain boundary plane) and driving force.*

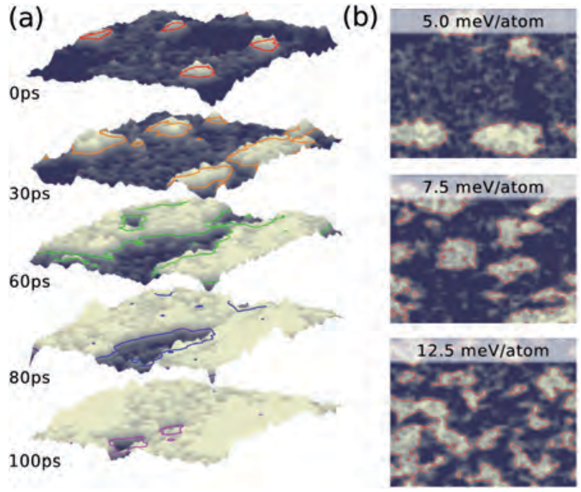

**Fig. 2:** *Snapshots of a migrating grain boundary surface for a large system (340 Å by 420 Å) with a driving force of 5.0 meV/atom at 600 K. (b) Snapshots of islands as a function of driving force.*

the size and energy of critically stable nuclei will decrease (Fig. 2b), explaining the upward curvature in the velocity with force.

We can model the excess free energy of an island nucleus of radius $r$ as

$$\Delta F(r,T,P_D) = 2\pi r(\gamma - T\sigma) - \pi r^2 dP_D$$

where $T$ is the temperature, $P_D$ the driving pressure, $d$ the height of the island, $\gamma$ the energy per unit length of the island edge and $\sigma$ the corresponding entropy density. We can obtain $\gamma = 31.5$ meVÅ$^{-1}$ from molecular statics calculations of relaxed islands (Fig. 3a). The edge entropy is modelled as $\sigma = \gamma/T_C$, where $T_C = 700$ K is the boundary roughening temperature. This model, free of fitted parameters, accurately predicts the shape of the Arrhenius curves of ln($v$) against 1/$T$ at varying driving force (Fig. 1b).

For migration by island nucleation and growth, the excess free energy of a critical island nucleus can be identified with the activation energy for boundary motion. This barrier will be $\Delta F^* = \pi\gamma^2(1 - T/T_C)^2/P_D d$. Crucially, we see that the activation energy has an inverse dependence on the driving force for motion. We have verified this inverse dependence with MD simulations at low driving forces (Fig. 3b).

Our simulation results and analysis reveal that the activation energy for the motion of smooth, flat grain boundaries is inversely proportional to the driving force. Realistic driving forces are typically around $10^{-3}$ meV/atom ($10^{-2}$ MPa), compared with a minimum of 1 meV/atom (10 MPa) accessible in simulations. Thus in the experimental (zero-force) limit the activation energy is infinite and the migrated grain boundary is never stabilised. An important and fully unexpected result of this study is that smooth, flat grain boundaries are thus immobile and the concept of an "intrinsic mobility" is meaningless. Of course, real grain boundaries are never perfectly flat: at high temperatures they become rough [1] and in all cases they contain structural defects such as extrinsic secondary grain boundary dislocations and steps [2]. Both effects remove the requirement for homogeneous island nucleation and so enable boundary migration.

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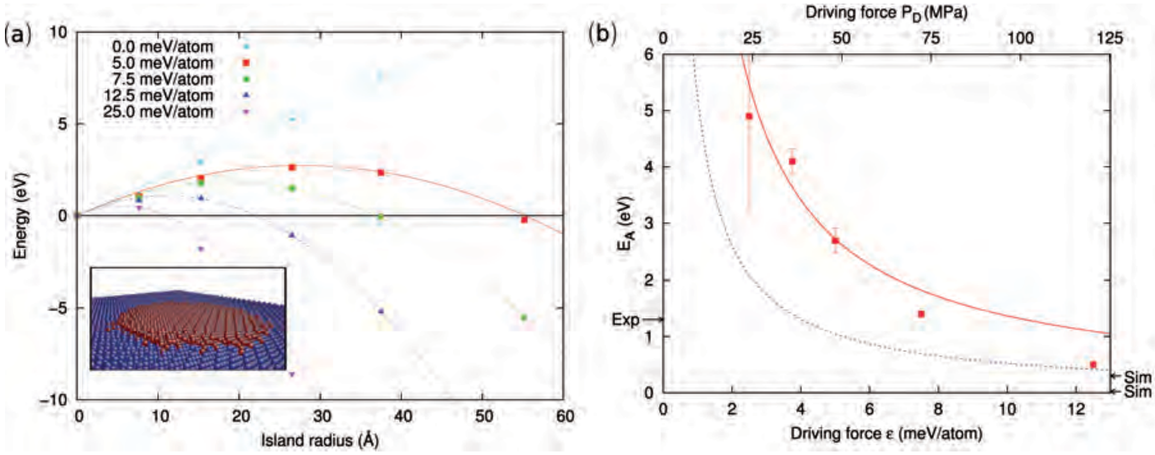

**Fig. 3:**. *(a) Nucleation barrier as a function of island radius. The symbols mark the results of static atomistic calculations using an EAM potential (see inset, island emphasised in red). The curves show the predictions of the simple model of island energy. (b) Activation barrier to form a stable nucleus as a function of the driving force. The symbols mark the energy barrier from boundary migration simulations; The red line shows the zero temperature free energy barrier F*(T = 0) predicted by the island model and the blue line an effective energy barrier at 550 K to enable comparison with literature benchmarks, shown on left and right axes.*

# Element-Resolved Corrosion Analysis of Fe-Based Bulk Metallic Glasses

*J. Klemm [1], M.J. Duarte [1,2], S.O. Klemm [1], A.M. Mingers [1], M. Stratmann [1], P.P. Choi [2], D. Raabe [2], K.J.J. Mayrhofer [1], F.U. Renner [1]*

[1] Department of Interface Chemistry and Surface Engineering
[2] Department of Microstructure Physics and Alloy Design

The complex elemental mixture in modern alloy systems often allows for extraordinary mechanical properties, but also constitutes a major challenge in corrosion science. Since all metals and compounds are fundamentally unique in their electrochemical behavior, the interactions between alloy constituents are decisive for the stability and applicability of materials. The individual role of each metal atom in macroscopic corrosion phenomena is important, and therefore requires element-resolved testing methods to fundamentally understand the underlying process. However, this element-specific perspective is strongly affected by the environment of metal atoms in the alloy. Under this aspect, particularly interesting are amorphous alloys or bulk metallic glasses (BMG) [1] which completely lack long range order [1,2]. This causes a perfectly homogeneous distribution of different elements in the matrix, an extremely rare feature in crystalline alloys due to the chemical segregation during phase formation.

In this study, the amorphous Fe-based model system $Fe_{50}Cr_{15}Mo_{14}C_{15}B_6$ was gradually crystallized by thermal heat treatment, characterized on the near-atomic scale by atom probe tomography (APT), and investigated with a novel element-resolved corrosion testing methodology in various states of crystallinity. This methodology allows following the effect of crystallization or chemical partitioning on the corrosion behavior and clarifies the element-specific dissolution, both being key challenges in modern corrosion science.

Fig. 1 shows the effect of an electrochemical corrosion test, where the samples were polarized for 1000 s in 0.1 M $H_2SO_4$ at each individual breakdown potential, on the surface topography of amorphous, partially nanocrystalline (620°C) and fully nanocrystallized (800°C) specimens. The amorphous sample only displays a minor change in topography (A). The partially nanocrystalline (620°C) surface demonstrates then a severe surface roughening on the nanometer length-scale. Finally, the fully nanocrystalline sample is covered by deep etch pits (C).

Phases with different elemental composition are evident from X-ray diffraction and APT, revealing local chemical changes in the material. To investigate the complex multi-element corrosion performance and clarify the topographic effects observed with atomic force microscopy (AFM), a micro-electrochemical scanning flow cell (SFC) [3] was coupled to a highly

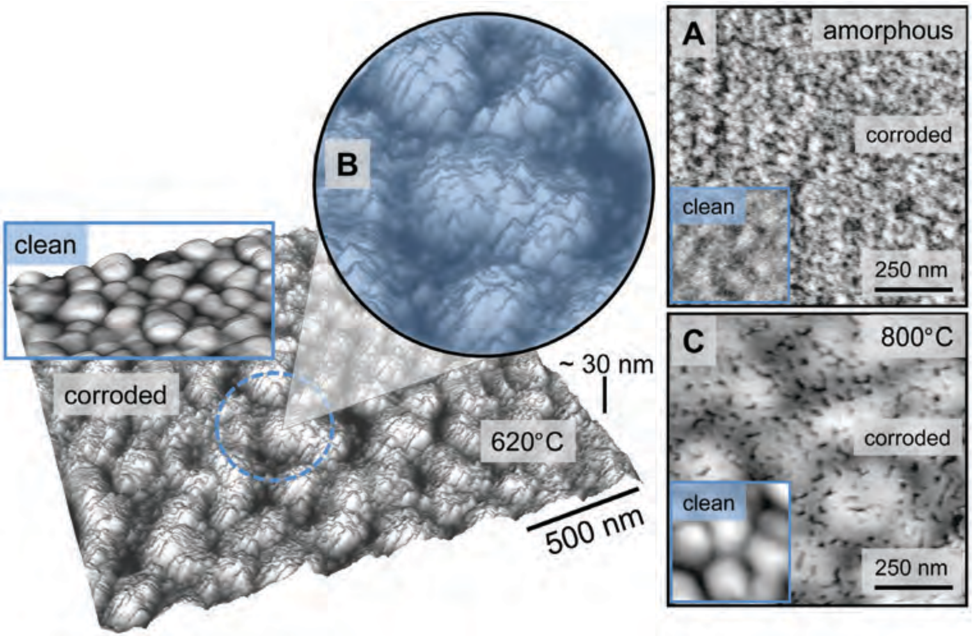

**Fig. 1**: *(A) AFM topography imagesof rough surfaces after corrosion test and corresponding clean surfaces (left corner, with blue edges) of (A) amorphous sample (B) 620°C sample (C) 800°C sample.*

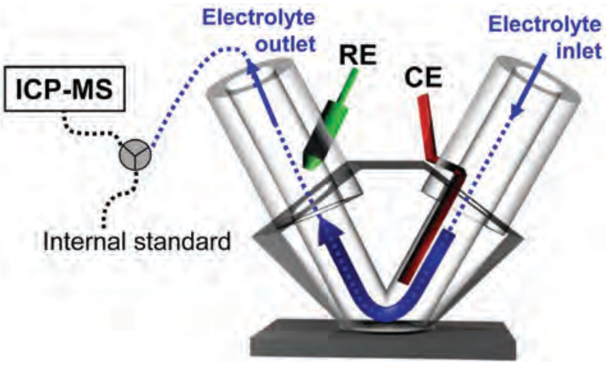

**Fig. 2**: *Schematic figure of the SFC coupled to an ICP-MS setup.*

sensitive ICP-MS (inductively coupled plasma mass spectrometry) [4,5] recording metal dissolution in real time. The setup is sketched in Fig. 2.

The corrosion behavior of the different alloys was investigated by linear sweep experiments in 0.1 M $H_2SO_4$ (Fig. 3 A-C black line). The results show a clear transition from a passive state limited by transpassive Cr dissolution (for amorphous and 620°C) to an early breakdown governed by Mo dissolution (for 800°C). The coupling of the SFC to the ICP-MS enables a direct comparison between the electrochemical (current density, $i_m$) and the analytical data (dissolution current density, $i_{Diss}$).The measured concentrations were converted into current density by application of Faraday's law [4,6]. The sum of all three individual elemental dissolution current densities, $i_{Diss,Me}$ with Me = Fe, Cr, Mo, (grey dashed lines in Fig. 3 A-C) show a good agreement with the measured current density $i_m$ for all three samples. Interestingly, significant changes are observed for the element-specific dissolution stoichiometry derived from the profiles, compared with the bulk material composition (Fig. 3 D-F).For the amorphous sample the main species dissolved is Fe with understoichiometric dissolution of Cr in the low potential range up to 700 mV, indicating enrichment of Cr at the outer passive layer. At higher potentials, i.e. the passive range, both Mo and Cr dissolve in equivalent ratio. An even higher contribution of Fe and Mo is observed in the sample annealed at 620 °C. Cr dissolves stoichiometrically only at the breakdown. At last, a very strong contribution of Mo approaching to the Fe signal is detected in the fully crystalline alloy, with Cr being distinctly minor.

The fully amorphous material thus shows chromium enrichment with low initial current densities. Accordingly, those surfaces remain comparably smooth. The partially crystalline alloy shows an enhanced dissolution of Fe and Mo throughout the polarization test, originating from Cr-depletion in the matrix confirmed by APT. The existence of nanoscopic, stable phases in a Cr-depleted matrix leads to a roughening, clearly observed in AFM. The etch pits observed for the fully crystalline samples however can be attributed to a Cr-depleted Mo-rich phase, which prevents passivity. The level of insights gained from element resolved corrosion tests and the synergies with other methods of surface science prove this concept to be highly valuable for modern corrosion research.

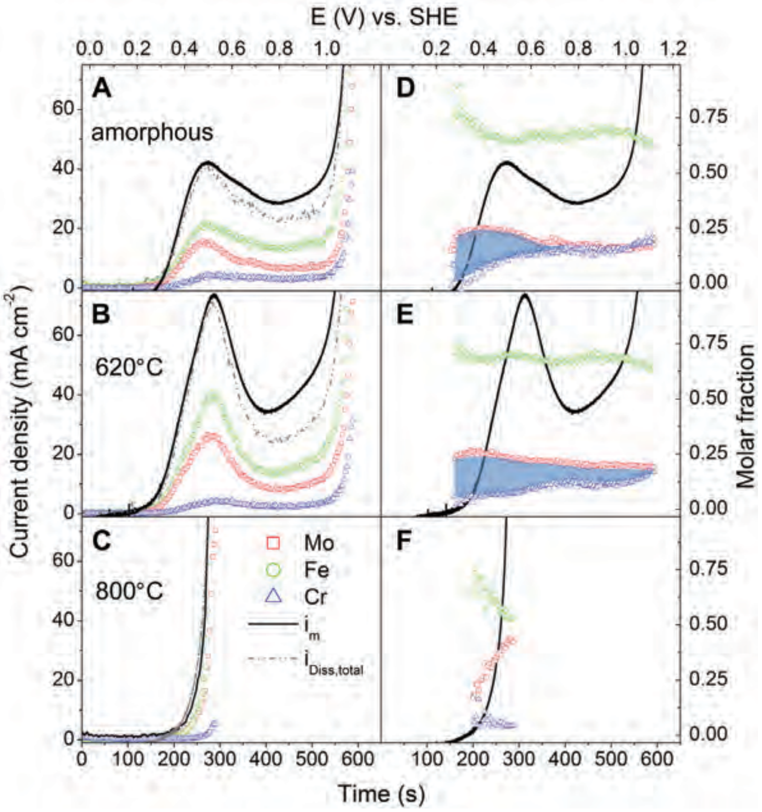

**Fig. 3**: (*A-C*)*: Potential sweep data $i_m$ (black continuous line) and online-ICP-MS dissolution profiles converted into dissolution current densities in 0.1M $H_2SO_4$ for the three samples. (D-F): Potential sweep data, $i_m$, with overlaid dissolution stoichiometry expressed as molar fractions of Fe, Cr and Mo. The difference between Mo and Cr dissolution is highlighted in blue (D-E).*

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# Surface Cracking on Cu−Au Surfaces

G.N. Ankah[1], D. Ma[2], M. Nellessen[2], D. Raabe[2], F.U. Renner[1]

[1] Department of Interface Chemistry and Surface Engineering, [2] Department of Microstructure Physics and Alloy Design

Cracking of structural materials is undoubtedly a very dangerous, often catastrophic issue in structural materials. For the understanding of the cracking behavior of materials the nucleation and initial growth is of special importance and often the decisive step for the evolution of a macroscopic crack. This is true on one hand, for cracking processes inside the bulk as it may occur during aging of materials. On the other hand many cracks initiate and start on the surface or the surface-near region as for example in the case of stress-corrosion cracking (SCC). Cracking is difficult to predict, both theoretically and experimentally. Typically, cracking events become only visible when they have already grown to a considerable size and the (atomic-scale) initiation and nucleation is not captured.

SCC is an often catastrophic failure process that occurs with specific alloys and environments that otherwise show a low corrosion rate. Many materials are susceptible to SCC but naturally high strength structural materials are of particular importance. Historically, the problem was observed in brass materials and Cu−Au alloys have been addressed as model systems for SCC in the last century. Although a longstanding topic in fundamental research there is no conclusive insight and many debates in the literature remain [1-3].

In this respect our recent discovery of microcracks on thiol-inhibited Cu−Au alloy surfaces during dealloying opens a promising way to address the cracking behavior and in particular crack initiation in alloys [4,5]. Compression studies using micropillars by Cynthia Volkert et al. showed active 111 slip modes in pure Au while nanoporous Au showed a foam-like behaviour [6,7]. Astonishingly the cracks on the thiol-modified $Cu_3Au$ surfaces possessed a nanoporous Au core with a clear sign of crystallographic fracture directions along the surface (Fig. 1). The different thiols used (from left to right) include benzeneselenol, hexadecanethiol (HDT) and mixed-aminobenzenethiol (m-ABT). The number of occurring cracks was observed to depend on the kind of initial surface treatment and the crack density varied strongly with surface orientation as shown in Fig. 2a (next page). Fig. 2b is a cross-sectional micrograph showing the morphology of one such crack within the nanoporous material.

The cracks that are observed might develop from the stressed ultrathin Au-rich film which then extends into the nanoporous material. The developing stress might be expected to be large since the thiol self-assembled films suppress the surface mobility of the Au atoms. In contrast to the localized corrosion of the inhibited systems, clean $Cu_3Au$ selectively dissolves

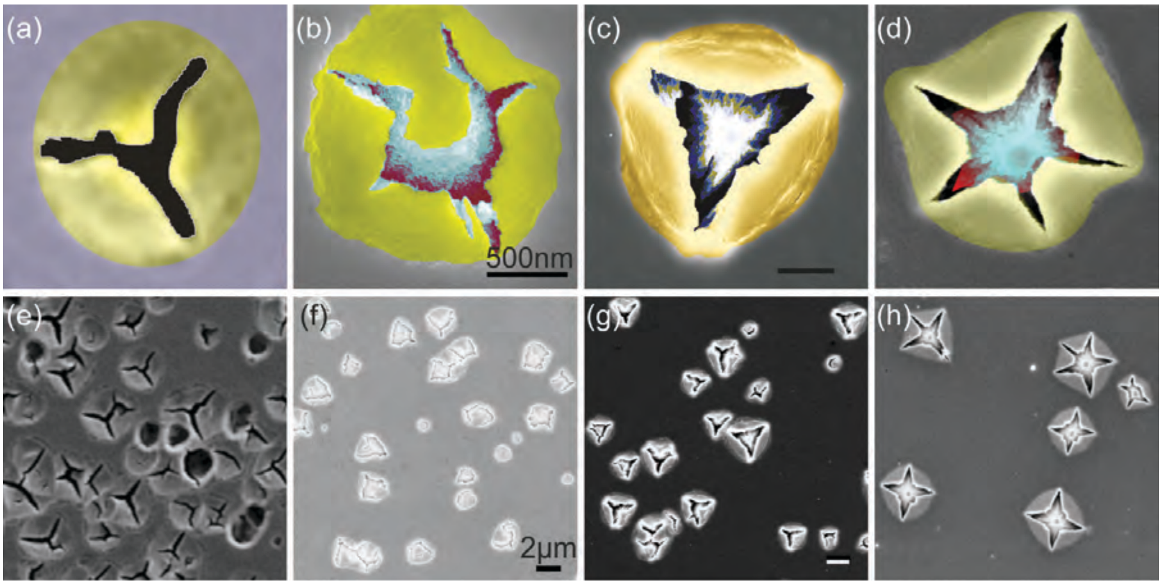

**Fig. 1:** *SEM images showing cracks on differently treated single and polycrystalline $Cu_3Au$ surfaces after dealloying in 0.1 M $H_2SO_4$: benzeneselenol (a and e), hexadecanethiol (b and f), and mixed-aminobenzenethiol (c, d, g and h) modified surfaces.*

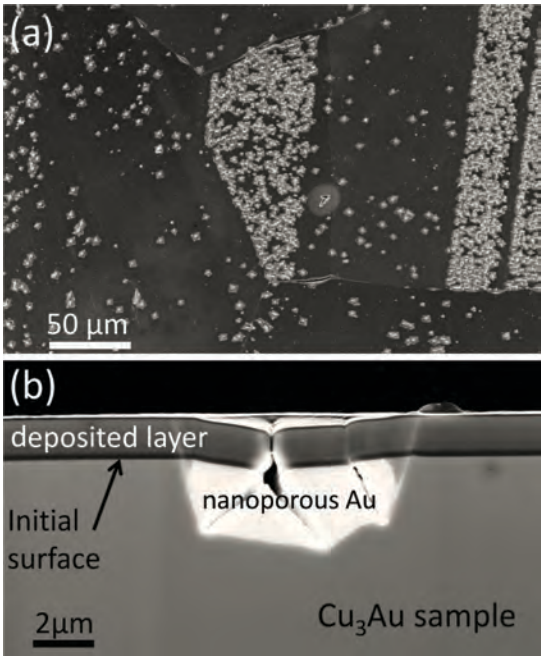

**Fig. 2:** *Scanning electron micrographs of a dealloyed $Cu_3Au$ polycrystalline sample. (a) Plane view showing grains with different crack densities. (b) Cross-section showing one specific crack that extends into the nanoporous material.*

and forms a homogeneous nanoporous structure. According to surface and cross-sectional analysis with EBSD, (110) grains were determined to have the highest density of cracks.

In a first step the stress development of the nanoporous gold and the $Cu_3Au$ matrix is described by a simple model solved by finite element method: we assume a half sphere will develop into porous Au from the surface of bulk $Cu_3Au$. The development of porous Au is mimicked by shrinking the half sphere down to 70% of its original volume. Anisotropic elastic properties are assigned to both porous Au and $Cu_3Au$. The crystallographic orientation of Au and $Cu_3Au$ are the same. For simplicity the ultrathin stacking reversed gold top layer is neglected. As shown in Fig. 3, during the shrinkage of the half sphere, stress concentration is built up in certain crystallographic directions. For instance, when (111) plane is parallel to the surface, the stress concentration will be in $[\bar{2}\,1\,1]$, $[\bar{1}\,\bar{1}\,2]$, and $[\bar{1}\,2\,\bar{1}]$ directions, where the elastic stiffness is the highest.

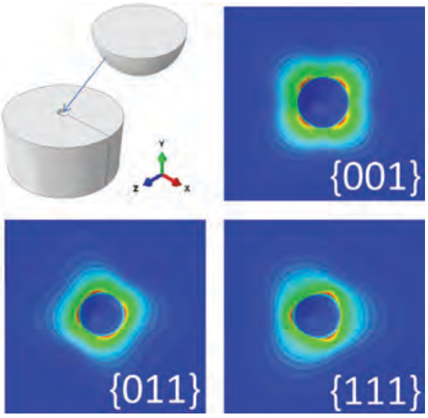

**Fig. 3:** *Von Mises Stress Contour plots showing the stress concentration distribution (color code: red is high and blue is low).*

Finally, the present work shows that the $Cu_3Au$ system evolves with "pronounced" microscopic failure when functionalized e.g. with thiol self-assembled films. This leads to a build-up of stresses, which are released abruptly hence generating cracks. Why the crack density is particularly high for the (110) orientated surfaces is still being investigated and one approach to better understand this effect is to conduct corresponding micromechanical simulations using an anisotropic elastic finite element model. Using a $Cu_3Au$ (111) single crystal, the crack tips with a common origin were found to follow a threefold rotational symmetry of the fcc-like $Cu_3Au$ (111) surface pointing to {110} cracks for selenole and {111} for thiol-modified surfaces. Many significant issues are still open for future research in this field of cracking during selective dissolution, including atomistic simulations, correlation with SCC, or a comparative study with other systems such as Cu−Pd or Ag−Au. The observed crack behavior in inhibited dealloying process as provided in this report may be of great importance to understanding crack initiation in general, especially if atomistic modeling contributes in establishing this concept.

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# Fundamental Studies on Novel Self-Healing Concepts for Corrosion Protection of Galvanized Steel

*A. Vimalanandan, T.H. Tran, M. Rohwerder*

Department of Interface Chemistry and Surface Engineering

Corrosion is a widespread problem with significant economic impact. Its consequences are also a loss of resources, energy, and the release of toxic substances to the environment. The latter aspect does not refer only to metallic cations (such as nickel) but also to corrosion inhibitors. Corrosion inhibitors are added to organic coatings applied for corrosion protection, the main measure for achieving efficient corrosion control for application in the automotive, aerospace, construction and appliances industries. The release of the inhibitors, however, does not occur in a controlled way. Instead, the inhibitors are continuously leached out of the coating. If corrosion in a defect occurs, they are then available for suppressing it. If there is no corrosion, they are fully released into the environment, continuously. Most of the current inhibitors are in discussion to be environmentally detrimental. Obviously, the best concept would be coatings that are capable of case triggered (i.e. only when corrosion occurs) release of active agents that stop corrosion and heal the corresponding defect (self-healing). Such coatings would not release great quantities of chemicals to the environment and still provide a superior corrosion protection. The idea of our research on intelligent corrosion protection is to develop coating systems that can do that. The best trigger is the change of potential. Conducting redox polymers are sensitive to changes in potential. However, their safe application for corrosion protection, especial on the technically very relevant zinc is a problem where the formation of an insulating layer leads to de-activation of the conducting polymer [1]. The research on developing reliable coating systems for intelligent release of active agents from conducting polymer is currently carried out within the framework of a DFG project (Heapocrates), in close cooperation with the Max-Planck-Institut für Polymerforschung (Prof. Landfester, Dr. Crespy). One of the main problems for achieving good self-healing is to store sufficient active agents for also closing defects larger than a pinhole. Synergy between components stored in the zinc coating, zinc cation themselves and components stored in the organic or hybrid inorganic-organic coating is the approach investigated in the framework of the MPG-FhG funded Project “ASKORR” in order to achieve this. As a first step synergetic effects between compounds stored in silica capsules in the zinc coating [2] with zinc cations released by zinc corrosion were investigated on exposed iron (defect down to the iron).

The zinc coating dissolves to protect steel while the oxygen reduction takes place on steel which causes a pH gradient on it. Close to zinc the pH is

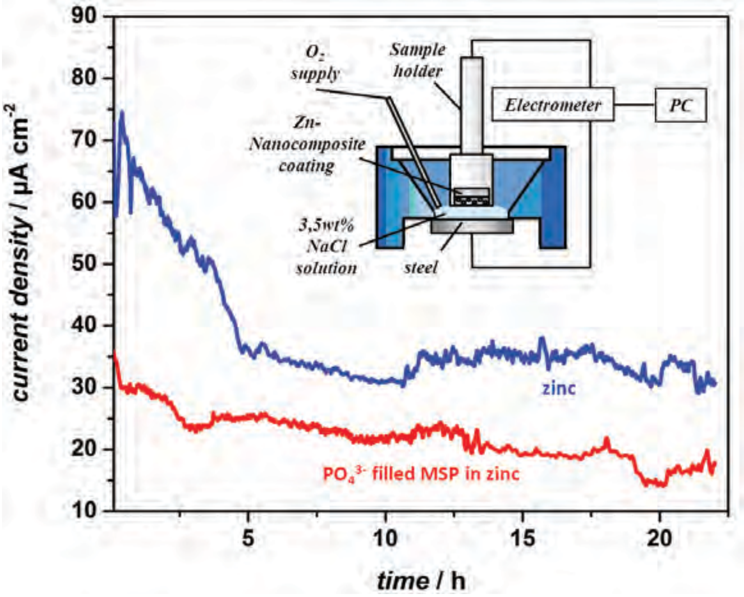

**Fig. 1:** *Experimental set-up for the galvanic current measurement and results showing the suppression of current density by phosphate loaded MSP embedded inside the zinc layer.*

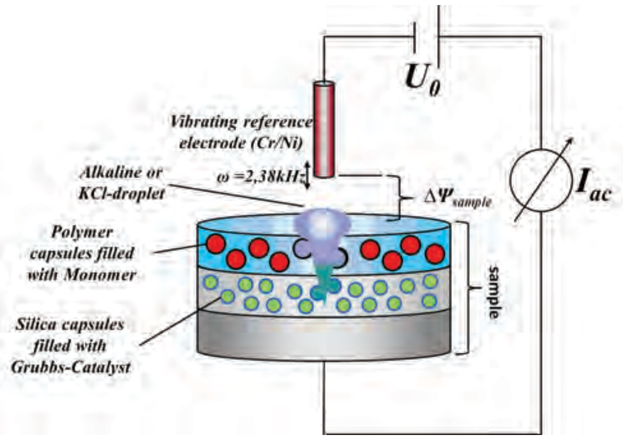

**Fig. 2:** *Experimental set-up of the self-healing experiments: the corrosion potential in the small scratch is monitored by Kelvin probe. Light blue: organic coating, grey: zinc coating.*

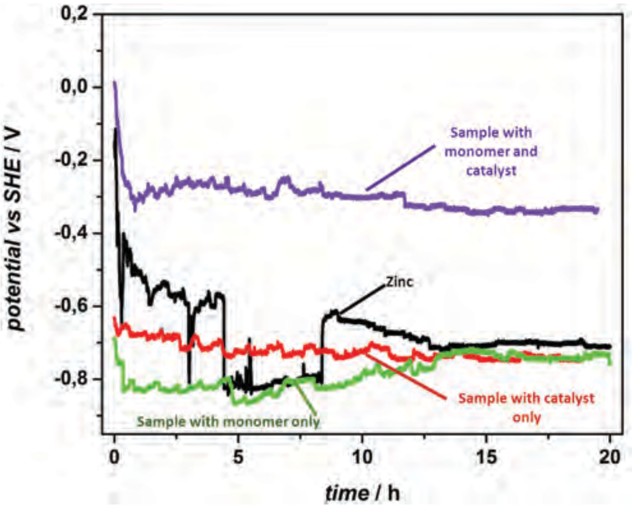

**Fig. 3:** *Proof-of-principle of the self-healing concept by polymerization. Only the sample with monomer and catalyst shows a self-healing behavior (passive potential). Reference measurements without or with just one component show constant active behavior.*

slightly acidic to neutral, further away the pH is highly alkaline. Hence, only at these alkaline pH the silica particles are dissolved and the stored inhibitors are released and can react with zinc cations to form a better protective corrosion product layer (see Fig. 1). The important point is: unlike release from classic pigments the release is delayed in time, by the diffusion of the capsules to the alkaline steel surface and hence the inhibitor is not consumed at the edge of the defect, where they are of little use, but right in the defect. This example shows how intelligent corrosion inhibition may be realized in future. However, full self-healing also requires the growth of a new organic coating in the defect. The best way is release of monomers and their targeted polymerization in the defect (and only there). This is done in the following way: polymerization catalysts are stored in silica capsules inside the zinc coating, where these reactive components can be stored for years without danger of de-activation by oxygen from the air. As they are released time-delayed, the monomers released from capsules in the primer have time to diffuse to the defect where the targeted polymerization will occur, leading to full coverage of the defect. One of the central topics of current research, in close cooperation with the project partners, is to find the optimal capsule systems for the primer: ideally conducting polymers or other redox active capsule materials should be used. In first test experiments, the capsule opening was just mechanically induced at the edge of the scratch through the coating. As in these experiments the amount of available active agents is very low (it should be higher, if release as a consequence of corrosion triggered delamination is triggered from a broader area surrounding the defect), experiments were focused on simulating atmospheric corrosion conditions where just a small amount of electrolyte is present at the defect. For this the experiments were controlled by Kelvin probe (see Fig. 2). After intense research and optimizing steps, successful self-healing was achieved (see Fig. 3). Better performance is expected when broader triggered release can be achieved by use of redox active capsules in the primer. Conducting polymer capsules modified by spacer groups to prevent deactivation are currently successfully developed in Heapocrates and additional redox active capsule materials tested within ASKORR.

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# Understanding the Mechanism of the Oxygen Reduction Reaction

*I. Katsounaros* [1], *W.B. Schneider* [2,3], *J.C. Meier* [1], *U. Benedikt* [2],
*P.U. Biedermann* [1], *A.A. Auer* [2], *K.J.J. Mayrhofer* [1]

[1] Department of Interface Chemistry and Surface Engineering
[2] Max-Planck-Institut für Chemische Energiekonversion, Department of Theoretical Chemistry, Mülheim an der Ruhr, Germany
[3] Ruhr-Universität Bochum, Center for Electrochemical Sciences, Bochum, Germany

The oxygen reduction reaction (ORR) is a fundamental reaction related to various disciplines such as energy conversion, material dissolution or biology. Recently, particular interest focused on its essential role in fuel cells or lithium-air batteries. However, the mechanism of the ORR on metal surfaces remains unclear. The distinction between the ORR mechanisms is based on the number of proton-coupled electron transfer steps that precede the O–O bond breaking step (Fig. 1). Among these mechanisms, hydrogen peroxide can be formed as an intermediate of ORR only by the 2nd associative mechanism. Indeed, hydrogen peroxide has been detected under certain conditions during ORR, but it remains unclear whether it is a key intermediate of the dominant ORR mechanism or a side-product [1]. A detailed understanding of the interaction of $H_2O_2$ with metal surfaces is essential on the road to understanding the ORR mechanism.

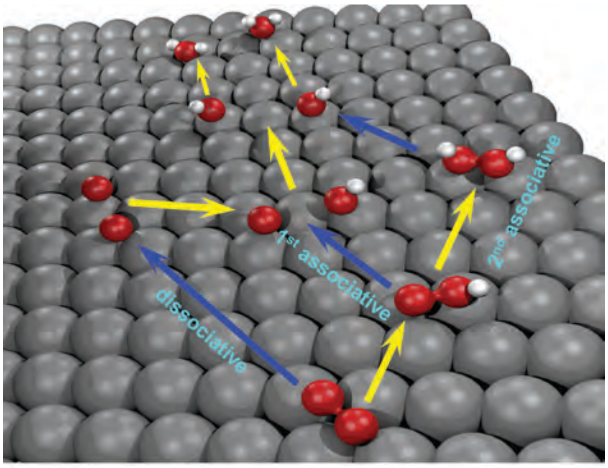

**Fig. 1:** *Proposed oxygen reduction reaction mechanisms.*

In weakly adsorbing electrolytes such as $HClO_4$, the total rate of $H_2O_2$ decomposition on polycrystalline Pt is controlled by mass transport, in the potential region between +0.2 $V_{RHE}$ and +1.5 $V_{RHE}$. In this region, the currents in the cyclic voltammograms (CVs) scale with the thickness of the diffusion layer and with the bulk concentration of $H_2O_2$ [2,3]. In addition, electrolysis experiments performed under potentiostatic conditions indicate that the rate of decrease of $H_2O_2$ concentration with time is diffusion-limited, regardless of the applied potential. This means that during ORR in such a system, $H_2O_2$ cannot be detected in the electrolyte even if it is formed at the interface. In a peroxide-containing solution, the potential-dependent Pt surface state triggers the corresponding reaction: Upon interaction with reduced surface atoms at low potentials, $H_2O_2$ adsorbs dissociatively producing $OH_{ads}$, while upon interaction with an oxidized surface at high potentials, $H_2O_2$ gets oxidized to $O_2$ by reducing the surface [3]. The measured current is the sum of the two partial currents restoring the thermodynamically preferred surface state at a given potential. Quantum chemical *ab initio* calculations (Fig. 2) showed that

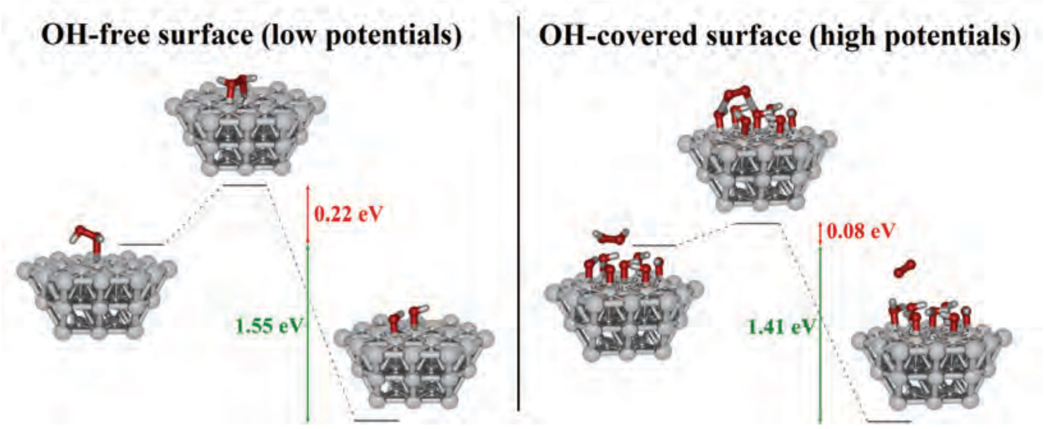

**Fig. 2:** *Energy diagram for the dissociation of $H_2O_2$ on a bare Pt(111) surface and for the oxidation of $H_2O_2$ on an OH-covered surface.*

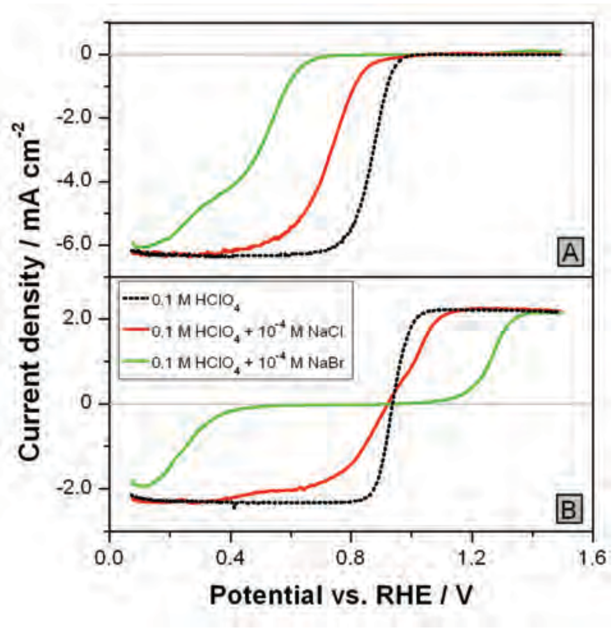

**Fig. 3:** *The impact of the halide ions on the background-corrected hydrodynamic voltammograms (1600 rpm) in (A) $O_2$-saturated electrolytes and (B) Ar-saturated electrolytes additionally containing 1x10$^{-3}$ M $H_2O_2$. Scan rate: 0.1 V s$^{-1}$.*

the activation barriers for either $H_2O_2$ dissociation or oxidation are easily overcome by the thermal energy and the reactions will proceed with a high rate at room temperature [2].

Therefore, the kinetics of both reactions of $H_2O_2$ dissociation (at low potentials) and $H_2O_2$ oxidation (at high potentials) are very fast as long as there is sufficient availability of platinum sites capable of carrying out any of the two reactions. This condition is fulfilled in weakly adsorbing electrolytes, where the coverage from inhibiting adsorbates is low. In particular, at potentials relevant to the ORR (i.e. below 0.95 $V_{RHE}$) the barrierless cleavage of the O–O bond of $H_2O_2$ is not prevented by the adsorption of inhibiting adsorbates.

The adsorption of halide spectator species limits the availability of sites that can break the O–O bond of $O_2$ and $H_2O_2$ [4]. The effect becomes stronger the higher the concentration of the halides in the electrolyte. Chloride adsorption inhibits the dissociative adsorption of $O_2$ more strongly than that of $H_2O_2$ (Fig. 3), implying that a larger number of adjacent Pt atoms is required to break the O–O bond of $O_2$, compared to $H_2O_2$. When a larger ion is added (such as bromide) the situation changes, and the inhibition of $H_2O_2$ reduction becomes stronger than that of $O_2$ (Fig. 3). This is because the O–O bond breaking is no longer possible for both $O_2$ and $H_2O_2$; however, there are still some single non-covered Pt atoms able to carry out the reduction $O_2$ to $H_2O_2$ without O–O bond cleavage. Therefore, depending on the extent of the inhibition of peroxide´s O–O bond breaking, the total rate of $H_2O_2$ decomposition may not be anymore limited by the mass transport of $H_2O_2$, which translates to a local $H_2O_2$ concentration higher than zero. In that case, during ORR under that conditions, the macroscopic detection of $H_2O_2$ as an intermediate of ORR will be possible at potentials where the coverage from the inhibiting spectators is sufficiently high.

In summary, $H_2O_2$ is unstable on Pt surfaces and it will immediately dissociate to OH if formed during ORR, unless the cleavage of the O–O bond is inhibited by adsorbed spectator species. The study of the interaction of $H_2O_2$ with Pt in conditions relevant to ORR, corroborates with previously reported data on the macroscopic $H_2O_2$ formation during ORR and can explain why hydrogen peroxide has been detected under certain conditions. Therefore, the differences in the proposed ORR pathways based on experimental data are an artifact and originate only from the changes in the interface structure caused by spectators.

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# Developing Design Principles for Stable Fuel Cell Catalysts by Studying Degradation Processes on the Nanoscale

J.C. Meier [1], C. Galeano [2], A. Kostka [3], V. Peinecke [4], F. Schüth [2], K.J.J. Mayrhofer [1]

[1] Department of Interface Chemistry and Surface Engineering
[2] Department of Heterogeneous Catalysis, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
[3] Department of Microstructure Physics and Alloy Design
[4] The fuel cell research center ZBT GmbH, Duisburg, Germany

Proton exchange membrane fuel cells are among the most promising technologies to replace traditional combustion engines and thus offer a clean and sustainable energy supply for automotive industry (if combined with renewable energy sources). The state of the art fuel cell catalyst is based on platinum nanoparticles dispersed on a carbon support, providing a high electrochemical active surface area (ECSA) of platinum to catalyze the oxidation of the hydrogen fuel at the anode, as well as the necessary oxygen reduction at the cathode. Under certain operation modes, however, the electrocatalyst limits the lifetime of a fuel cell. Particularly on the cathode side during start up and shut down the catalyst faces most drastic conditions such as low pH values, elevated temperatures, high potentials as well as harmful potential fluctuations. As a consequence the catalyst degrades over time, resulting in a decrease in platinum surface area and a loss in overall performance of the fuel cell [1,2].

One major obstacle in the design of catalysts with improved stability is the lack of knowledge about the underlying degradation processes of fuel cell catalysts on the nanoscale. To address this issue we developed the identical location approach for transmission electron microscopy (IL-TEM) [3-5]. IL-TEM visualizes the same catalyst location before and after an applied degradation protocol, which has not been accessible before. An example of a catalyst location studied via IL-TEM is shown in Fig. 1.

Moreover, the identical location approach has been extended also to other electron microscopic techniques such as SEM, or even electron tomography, which add complementary information to a standard IL-TEM experiment [5]. While TEM only provides a 2D projection of a three-dimensional object, IL-tomography can visualize changes in a catalyst material due to an electrochemical aging test in 3D. An IL-tomography representation of a Pt/Vulcan catalyst is visualized in Fig. 2C and 2D (see next page) and compared to standard IL-TEM images of the identical catalyst location (2A, 2B). Particle growth due to agglomeration as well as detachment can be clearly observed for the standard Pt/Vulcan material. Additionally the breaking off of a complete carbon fraction from the catalyst aggregate was visualized. This carbon fraction was originally connected to the main aggregate via small carbon bridges, which corroded during the simulated start-stop conditions [6].

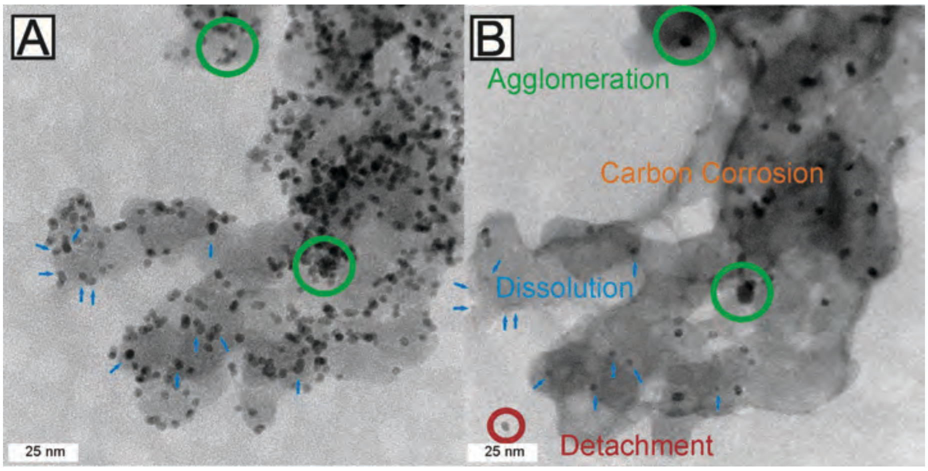

**Fig. 1:** *IL-TEM micrograph a Pt/Vulcan catalyst before (A) and after (B) 3600 potential cylces between 0.4 and 1.4 VRHE in 0.1 M HClO4 at 1 Vs-1. Several overlapping degradation processes can be observed: Green circles indicate particle growth, the red circle highlights a detached particle, blue arrows point at dissolving particles (printed from our publications [6] with permission of ACS Catalysis).*

The knowledge about the strong contribution of detachment and especially agglomeration to the overall degradation of the standard Pt/Vulcan catalyst during start-stop – as disclosed by IL-TEM and IL-tomography – was applied in the design of a more stable catalyst. Namely, a hollow graphitic carbon sphere support (HGS) with a three-dimensional interconnected mesoporous network was synthesized and loaded with platinum. After a thermal treatment step a highly stable fuel cell catalyst with platinum particles in a size range of 3-4 nm incorporated in the mesoporous structure (Pt@HGS$_{900°C}$) is obtained. Measurements in an electrochemical half cell demonstrated standard activity and superior stability for this material. *In situ* fuel cell tests confirmed the results

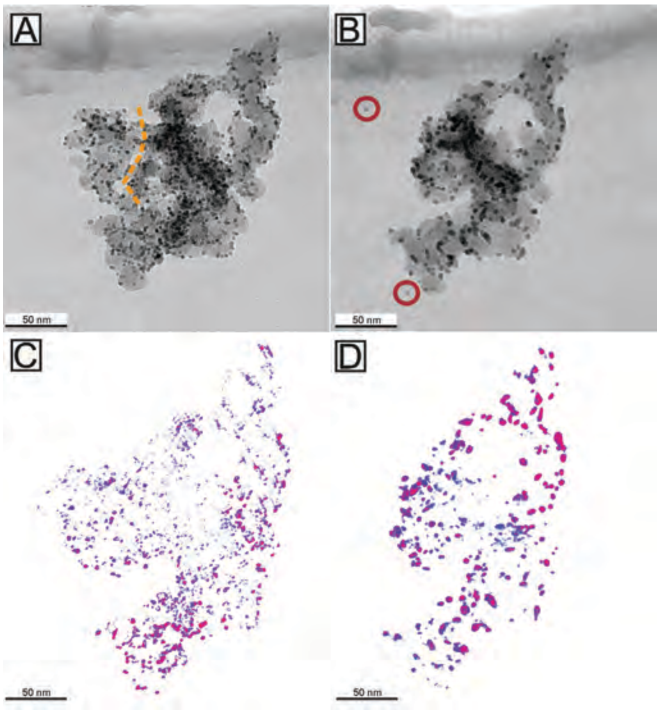

**Fig. 2:** *IL-TEM micrographs (A, B) and IL-tomography images (C, D) of Pt/Vulcan before (A, C) and after (B, D) 3600 potential cylces between 0.4 and 1.4* $V_{RHE}$ *in 0.1 M* $HClO_4$ *at 1* $Vs^{-1}$ *(printed from our publication [6] with permission of ACS Catalysis).*

of the half cell measurements: Pt@$HGS_{900°C}$ exhibits only minor losses in the cell voltage and therefore a superior stability under start-stop conditions compared to Pt/Vulcan, making it a highly promising material for application in real fuel cells.

Fig. 3A and 3B are an overlap of IL-SEM micrographs (green color) and IL-STEM micrographs (red color) before (3A) and after (3B) an accelerated aging test. The test reflects the high stability, as the HGS spheres stay intact and only few platinum particles are lost after electrochemical treatment. In contrary to the Pt/Vulcan catalyst no signs of agglomeration can be observed as the average particle size does not change. Particles on the surface of the spheres, which are not protected by the porous network are observed to vanish preferentially after the degradation test, while in total only about 14% of all particles are lost. Based on the combined IL-SEM and IL-STEM investigations it can be stated that particles located within the mesoporous network are stabilized as they are less likely to detach and agglomerate. This proves that stabilization due to confinement of platinum particles in a mesoporous network can be a valuable strategy to design more robust electrode materials.

In this study insights from IL-TEM and IL-tomography into catalyst stability were successfully employed for the synthesis of a more stable catalyst, which opens new perspectives for a more systematic design of stable electrode materials.

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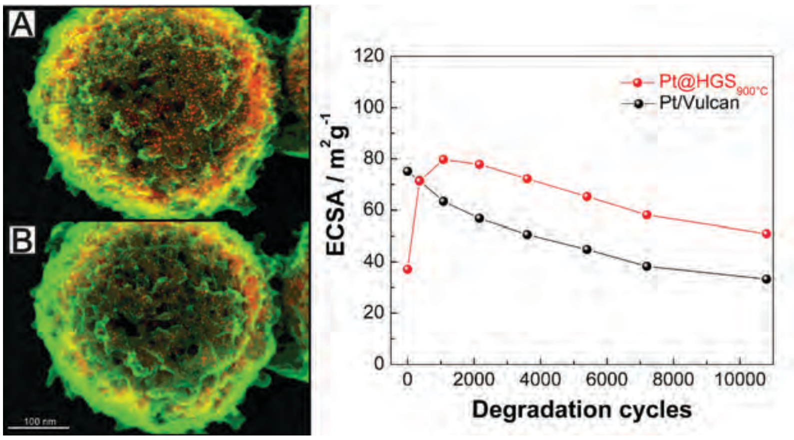

**Fig. 3:** *A is an image before, B after 3600 degradation cycles. A and B each show a complete carbon sphere. For both images a SEM micrograph (green) and STEM micrograph (red) were overlapped. The graph on the right demonstrates that Pt@*$HGS_{900°C}$ *is able to maintain a higher ECSA during an accelerated degradation test compared to Pt/Vulcan.*

# *In situ* Investigation of Oxide Thin Film Evolution on Zinc

*Y. Chen, P. Schneider, A. Erbe*

Department of Interface Chemistry and Surface Engineering

Zn is one of the most important metals in applications. Due to its oxidation propensity, Zn is a very efficient sacrificial anode in cathodic protection, and used as metallic coating [1,2]. Corrosion products of Zn metal and its coatings normally include ZnO, $Zn(OH)_2$ and carbonates [1]. The electronic properties of the mostly semiconducting oxide layer have been found to play an important role in the corrosion behaviour of Zn [1,2]. Electronic structure calculations can be used to obtain detailed insight e.g. into the role of defect in different crystalline materials. On the other hand, they need to be complemented by experimental investigation of properties, such as thickness and band gap. The particular challenge in case of thin films forming in the initial stages of corrosion processes is that they are highly disordered, transient species. Formation and evolution of such structures can be conveniently analysed using optical reflection spectroscopy, as the optical absorption spectrum is directly related to the electronic structure of the film. Here, spectroscopic ellipsometry has been used to study the initial stages, as well as the evolution with time, of layer thickness and layer absorption spectrum, in controlled atmospheres and in electrolyte [3-5].

A novel method, based on a perturbation analysis [6], has been developed to extract the thickness without the need for an optical model for a layer with a thickness much smaller than the wavelength [5]. As the optical constants of zinc in the ultraviolet to visible spectral range behave Drude-like, light absorption from an ultrathin layer affects mainly the modulus of the amplitude reflection coefficient $r_p$ for p-polarised light. The amplitude reflection coefficient $r_s$ for s-polarised light is almost unaffected. As the ellipsometric experiment measures $r_p/r_s$ = tan(Y) exp(i D), with i denoting the square root of -1 and the two experimental angles Y and D, a lower value of tan(Y) (or Y) compared to the metal without layer or with a non-absorbing layer follows [4]. This behaviour is demonstrated in Fig. 1.

Further, SE was used for *in situ* investigations of the Zn/electrolyte interface during both potentiostatic (chronoamperometry, CA) and potentiodynamic (cyclic voltammetry, CV) treatments of Zn in alkaline carbonate solution. During CV, the thinning of the oxide in the negative scanning and subsequent growth of oxide in the reversed positive scanning on Zn can be followed in a CV-like manner (Fig. 2).

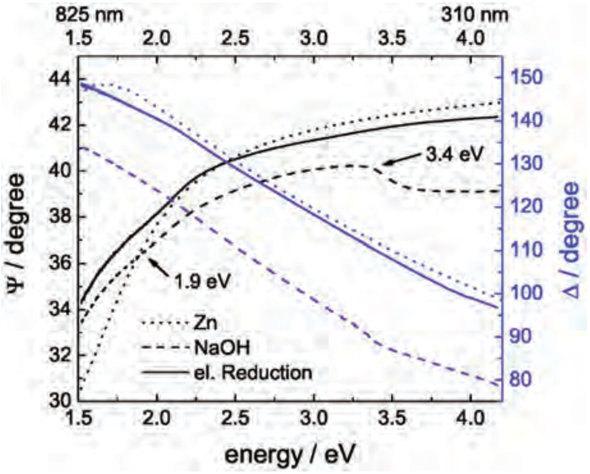

**Fig. 1:** *Ellipsometric spectra of zinc (dotted lines, simulated data on the basis of literature data). Treatment in NaOH (dashed lines) yields a layer with a thin oxide film, where the main electronic absorption of ZnO is visible as a downwards bend in Ψ. Electrochemical reduction results in a substantially different kind of oxide, judging from its light absorption characteristics.*

In the potential regime where the surface is oxide-covered, the layer thickness increases/decreases linearly with potential in anodic/cathodic scans, as reported for passive materials. Moreover, a rapid decrease/increase in the layer thickness in the reduction/oxidation peak has been found. Analysing the integrated currents show that oxide growth is accompanied by metal dissolution [5]. Future experiment in cooperation with experiments developed in the Electrocatalysis group should show more details about the relation between oxide formation and metal dissolution.

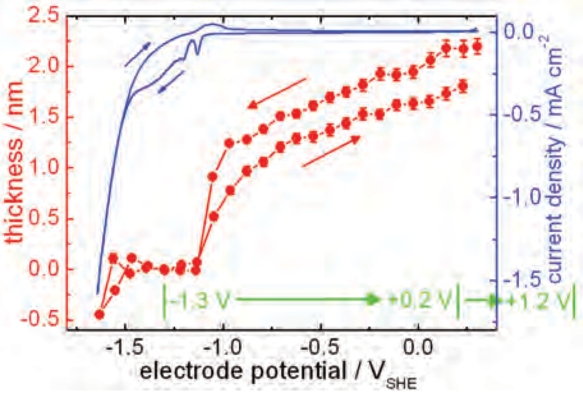

**Fig. 2:** *CV (blue) and ellipsometric thickness cyclic voltammogram (red) of zinc in 1 M $Na_2CO_3$ at 2 mV/s.*

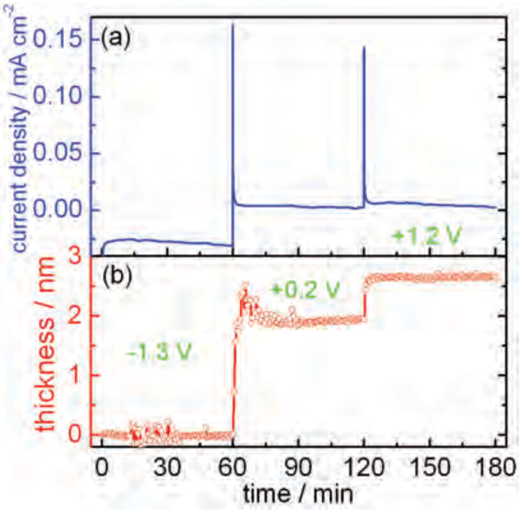

**Fig. 3:** *Current densities (a) and oxide layer thickness (b) as result of chronoamperometric experiments with potential jumps. Electrode potentials were -1.3 V (0-60 min), +0.2 V (60-120 min) and +1.2 V (120-180 min).*

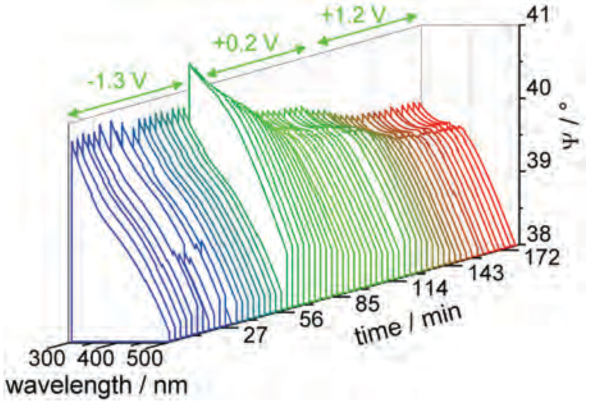

**Fig. 4:** *Spectra of $\Psi$ during chronoamperometric experiments with potential jumps at 60 min and 120 min (as in Fig. 3). At the initial potential of -1.3 V, no oxide absorption is visible. After the first and second potential jump (to +0.2 V and +1.2 V, respectively), the slow development of the ZnO absorption at 360 nm (3.4 eV) is clearly visible.*

In the CV-type of experiments, an inspection of the layer absorption shows a behaviour which can only be understood as being due to changes with time, rather than due to changes with potential. Therefore, potential jump experiments were performed from a potential in the oxide-free region (-1.3 V), to a potential in the oxide-covered region (+0.2 V), followed by a second jump to +1.2 V. The resulting current show a spike after the potential jump (Fig. 3a) while the thickness jumps to almost its final value within the first minute after the potential jump (Fig. 3b). On the other hand, Fig. 4 shows only a slow evolution of the electronic absorption of ZnO over ~30 min, before it remains constant until the next potential jump. Overall, these results show that the oxide layer takes time to mature. An initially formed layer is transforming slowly into ZnO. In the second phase of the layer evolution after 30 min, metal dissolution is still occurring, at a constant absorption spectrum (and hence, electronic structure) of the oxide layer. The kinetics of the layer evolution is independent of the electrode potential itself, as it behaves the same at +0.2 V as at +1.2 V [5].

While in carbonate electrolyte, the layer evolves to its final thickness faster than in 1 min while the electronic ZnO absorption evolves over ~30 min, the opposite behaviour is found when monitoring the oxide growth in argon, oxygen and air atmospheres of different humidities [4]. During atmospheric oxidation of zinc, the electronic absorption develops faster than the layer thickness. Interestingly, the oxide absorption is also fully developed after ~30 min, as in solution. The oxide layer thickness does, however, grow over hours even in argon. While oxide growth slows down with time, in most atmospheres now limiting behaviour of the growth is observed [4].

The two independent time scales for growth and ZnO electronic structure formation may be specific to zinc, which may form initial hydroxides. These hydroxides can slowly condense to finally form ZnO. On the other hand, such behaviour may be more general. Currently, oxide growth on other metals in investigated, with the aim of understanding charge transport through the layers, and the follow-up chemical reactions of the layers.

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# Self-Assembled Monolayers on Metals and Metals on Self-Assembled Monolayers

*M.I. Muglali* [1], *P. Koelsch* [2], *A. Erbe* [1], *M. Rohwerder* [1]

[1] Department of Interface Chemistry and Surface Engineering
[2] University of Washington, Seattle, USA

Self-assembled monolayers (SAMs) on metals can be used as low molecular models for polymers on metals. For studies of the metal/organic interface, they offer the advantage of a well-defined linkage between organic material and metal, as well as the well-known atomistic/molecular structure on both sides of the interface. Based on the long-term experience in surface modification and electrochemistry, we have investigated reactions at SAM/metal, as well as at metal/SAM interfaces in electrolyte. Electrochemical desorption/readsorption studies reveal important results concerning the nature of the interfacial interactions between a chemisorbed monolayer and a metallic substrate, besides defining the applicable potential range for SAM modified electrodes. These reactions can be seen as a molecular model for the destruction of a metal/polymer interface. Besides, they define the limit of applicability of SAMs.

Here a full investigation was carried out of the physical state of the desorbed molecules, and reactions concurrent to desorption, by combining spectroscopic techniques with electrochemistry. For these studies, Au(111) substrates have been modified by the highly ordered monolayers of 4-(4-(4 pyridyl)phenyl)phenylmethanethiol (PyPP1) [1]. The electroreductive desorption of PyPP1 SAMs shows unusual features in cyclic voltammograms (CVs). In alkaline solutions, the desorption behavior of the PyPP1 on Au is characterized by multiple reductive peaks in CVs. These peaks are, however, exceptionally large and contain one order of magnitude larger currents than expected for a simple desorption reaction (CV in Fig. 1). Based on rotating ring-disk electrode measurements, the origin of these excess currents have been found to be a concurrent rapid hydrogen evolution reaction (HER). The catalyzed HER currents appear as another peak in CVs, subsequent to thiol desorption. Confirmation of this phenomenon by *in situ* ellipsometric measurements hints to a transport mechanism in the electrochemical double layer region. *In situ* sum frequency generation (SFG) spectroscopy experiments (Fig. 1a) on PyPP1/Au(111) samples have demonstrated that PyPP1 SAMs preserve their two-dimensional order near Au during and even after the reductive desorption. Linking the voltammetric and spectroscopic results, a model was developed as shown in Fig. 1c, involving a structuring of water in the nanometer-sized reaction volume between desorbed SAM and Au electrode, by the structurally extremely stable monolayer, leading to the observed catalysis of the HER [2].

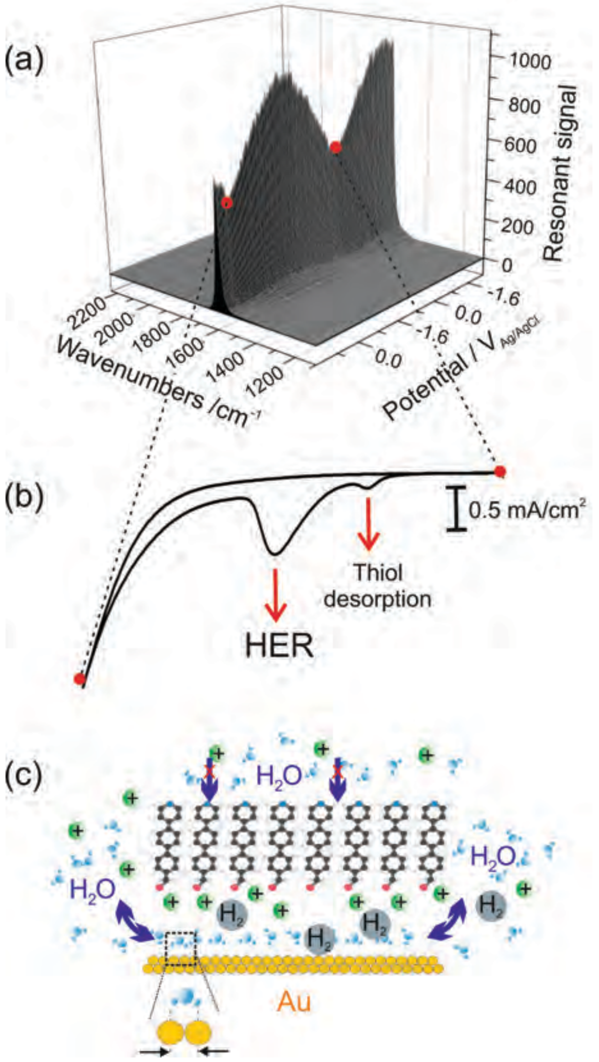

**Fig. 1:** *(a) SFG spectra of the pyridine ring vibration of PyPP1 on Au(111) during 1 1/2 CV cycles covering the reductive desorption potential of the SAM. No loss in order is observed at the desorption potential. (b) Cathodic peaks marking the reductive SAM desorption and associated rapid HER in a CV. (c) Schematic illustration of the proposed desorption mechanism. HER is catalyzed through optimum orientation of water molecules inside the gap between the desorbed crystalline thiolate film and the Au surface.*

In many cases, the actual use of SAMs bases on reactions occurring on the organic film. One specific case for such applications is the metallization of

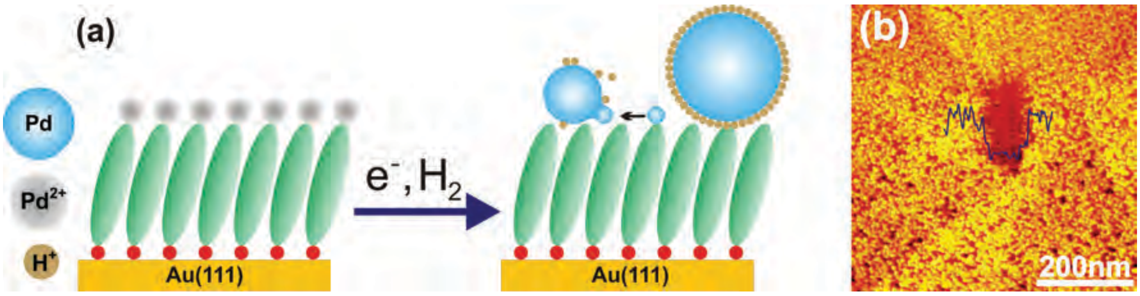

**Fig. 2:** *(a) Schematic illustration of metallization process through reduction by $H_2$ reduction of the SAM-coordinated $Pd^{2+}$ ions. (b) Scanning tunnelling microscopy (STM) image of the deposited Pd adlayer with full coverage. The interaction between SAM surface and Pd nanoclusters becomes weak after $H_2$ adsorption. This weak interaction enables a displacement of the nanoclusters with the STM tip as demonstrated in the center of the image after repetitive scans.*

SAM surfaces, needed for the development of metal/organic/metal junctions for organic electronics. However, the deposition of a top metallic layer onto a SAM is rather challenging.

For Pd deposition onto the well-characterized PyPP1 surfaces, we have demonstrated two strategies. The first one involves an electrochemical method [3], which has been the subject of several studies [4]. Further, a new electroless metallization method was introduced. This method bases on the reduction of the metal ions coordinated at the SAM surface by exposure to $H_2$ [5]. Its mechanism is schematically sketched in Fig. 2. The focus was on understanding the details of the deposition process. For instance, complexation kinetics of metal ions at the pyridine-functionalized SAM surface is discussed as a decisive process for understanding the coordination mechanism prior to the reduction step. Moreover, for the case of metallization by Pd, hydrogen adsorption on Pd during the reduction step has been studied. In agreement with theoretical work, there is a strong interaction and modification of Pd adlayer through adsorbed hydrogen [6], for which experimental evidence is provided.

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# Early Stages of High Temperature Corrosion in Steel Processing and Manufacturing

*M. Auinger, A. Vogel, D. Vogel, M. Rohwerder*

Department of Interface Chemistry and Surface Engineering

High temperature corrosion represents a vitally studied research field and fundamental understanding of the underlying mechanisms of material degradation is still a necessity to face upcoming challenges in modern energy politics.

Our current research activities in this field aim on a better understanding of the early stages of material degradation, especially on the changes of the surface conditions of the material under investigation. Many efforts have been undertaken to establish an accurate definition of process parameters to generate well-characterized exposures for a large variety of experimental possibilities.

Besides the unique combination at our institute, which makes this laboratory one of the flagship places in high temperature research worldwide, it amalgamates the benefits of rapid heating up to 30 °C $s^{-1}$ (due to the use of an infrared-furnace), an oxygen impurity content of the used reaction gases below 3 ppm and a long-term stable dew-point (±0.2 °C). Thus the high temperature lab allows experiments covering a wide parameter field.

However, the *in situ* measurement of mass gain, especially during fast temperature cycles, which is a problem of significant practical importance, remained a problem that was experimentally unsolved. The reason for this is that due to fast changes of temperature in close vicinity to the sample surface, thermal drifts begin to dominate the thermobalance signal, making a clear scientific interpretation of the mass changes impossible. This problem is well known to the community for more than a couple of decades but a sound solution of such an issue has never been presented so far. Instead, trials to combine fast heating by infrared furnace with thermobalance were so far unsuccessful, i.e. results obtained with set-ups caused a lot of doubts and controversies and hence this combination is up to now only used for long-term exposures of several hundred hours.

In addition to coupling of IR-heating and thermobalance, it was therefore decided at MPIE to eliminate the content of inert gas – which often represents up to 95 % of the atmosphere – and to perform thermal exposures in a low pressure environment instead. By

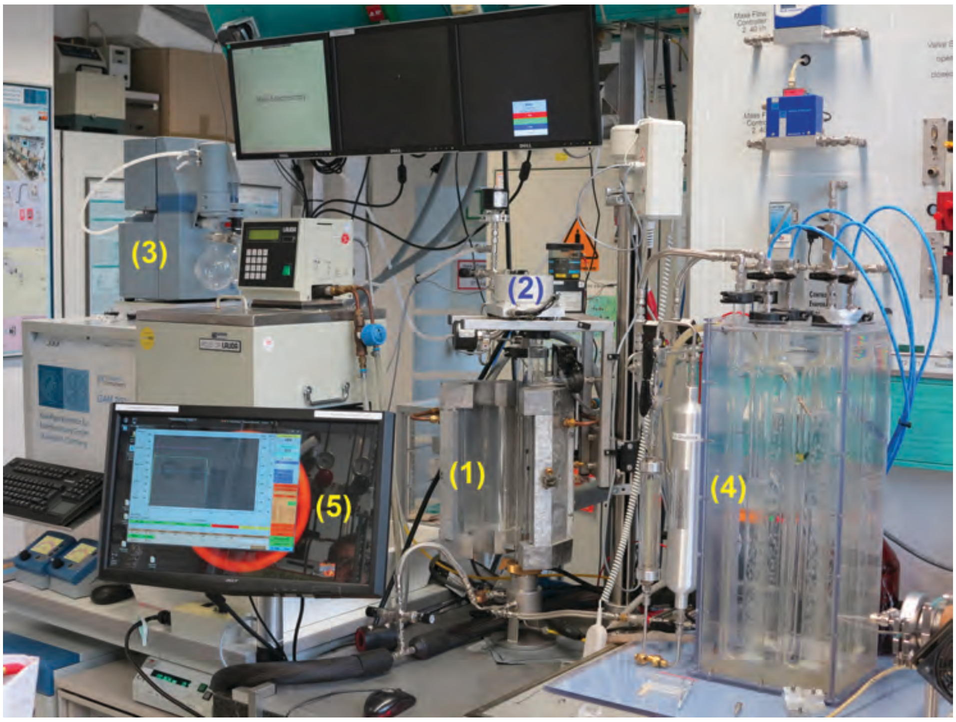

**Fig. 1**: *View of the novel thermobalance set-up for fast measurements showing an IR furnace (1) with thermobalance (2), a vacuum pump for adjusting the low-pressure conditions (3), gas humidification (4) and computer display for measurement results (5).*

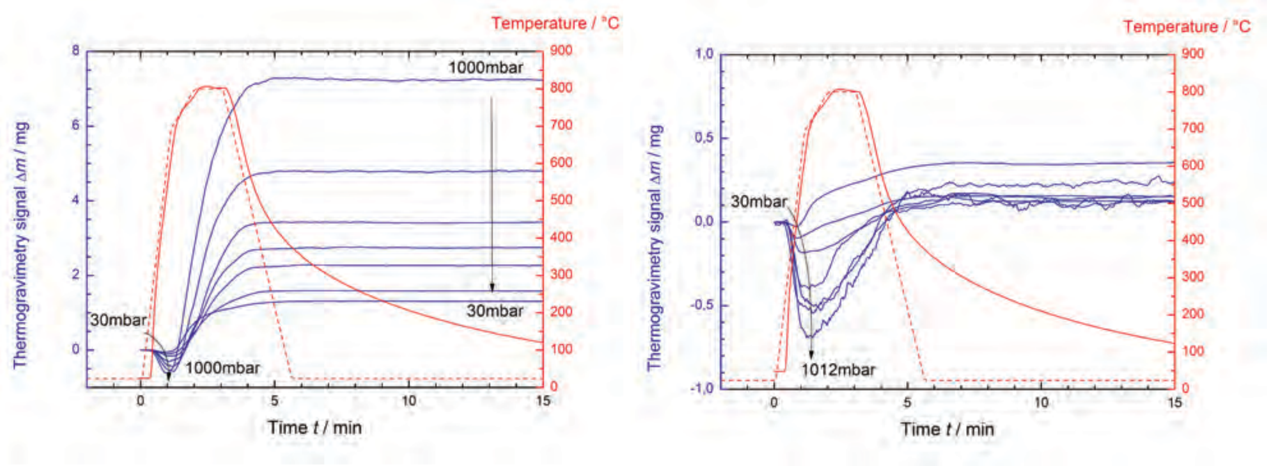

**Fig. 2**: *Pressure dependence of the thermogravimetric signal during a fast heating process in stationary argon atmosphere (left) and with continuous gas flow of 20 l h*$^{-1}$ *(right).*

this produce, we can still establish the same amounts of all reactive components and reduce the buoyancy effects by more than a factor of 10.

Initial tests with exposures of pure iron samples in an argon atmosphere, as illustrated in Fig. 2, prove the success of this technique. Whereas in both experiments a clear reduction of the initial drop in the recorded mass signal has been observed, the fluctuations in a steady gas flow could also be reduced by several orders of magnitude. This enables extremely accurate measurements of *in situ* mass changes down to 0.1 µg. Please note, that a low oxygen contamination in the argon gas causes a residual mass increase and that this can be clearly seen at 30 mbar (Fig. 2, left), whereas this is not possible at ambient gas pressures.

This method provides a unique contribution to elucidate the kinetics of oxidation in the early stages and closes the gap between experimental observations on a large time scale and other measurements of the initial stage behavior. Hence this technique represents an important scientific progress in the field and helps to shed light on early stage material degradation, both from a scientific point of view as well as for many industrial processes.

# Biological D-Surface Structure: A Lesson from Nature on Photonic Crystals Design

X. Wu [1], A. Erbe [2], H. Fabritius [1], P. Ebbinghaus [2], M. Stratmann [2], D. Raabe [1]

[1] Department of Microstructure Physics and Metal Forming
[2] Department of Interface Chemistry and Surface Engineering

In the near future, photonic band gap materials are expected to play the same important role in photonics as semiconductors do in electronics [1]. Biological photonic crystals, particularly those of insects with their ability to display beautiful colours [2], provide models to learn the principles used by nature to open up photonic band gaps [3]. The small scales covering the beetle *Entimus imperialis* (Fig. 1a) are subdivided into irregularly shaped domains that mostly show striking colors, yet some appear transparent. Exposure of the photonic crystal using focussed ion beam (FIB) milling reveals that the photonic crystal is a bicontinuous cubic structure, where space is divided into two continuous subvolumes, namely, cuticular network and an air phase (Fig. 1b). The two phases are separated by a triply periodic intermaterial dividing surface (IMDS) generating a D-surface structure. Different observed colours correspond to different orientations of the same photonic crystal in each domain (Fig. 1b), making every scale act like a photonic polycrystal. Transparent domains contain the same structure as colored ones, but the air phase is substituted by a second solid phase (Fig. 1b). Transmission Fourier transform infrared (FTIR) spectra reveal the presence of two strong peaks at 1020 and 1091 cm$^{-1}$ in transparent domains, which are typical for the most abundant four-fold coordinated silicon in $SiO_2$ [4] (Fig. 2). Together with the strong silicon peaks in energy-dispersive X-ray (EDX) spectra of transparent domains, this indicates that the beetle incorporates $SiO_2$ into its scales, which has never been observed before.

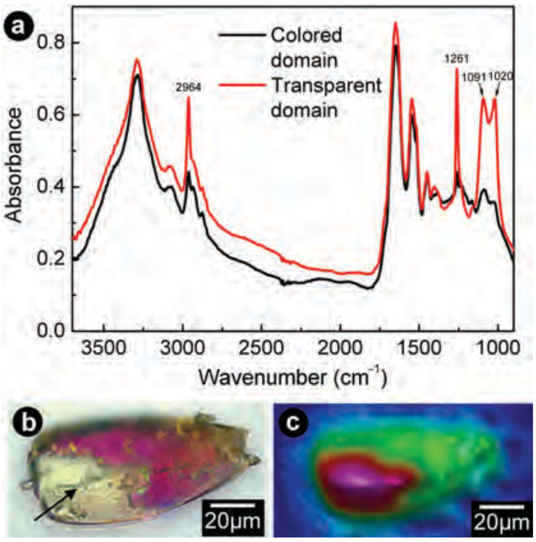

**Fig. 2:** *(a) Transmission FTIR spectra of the transparent (red line) and coloured (black line) domain. (b) Light micrograph of the analysed scale (arrow: transparent domain). (c) Spatial distribution of the integrated absorbance from transmitted light of the Si-O stretching mode spectral region (blue: weak integral absorbance, purple: strong integral absorbance).*

Using high-resolution scanning electron micrographs of all exposed domains, we morphometrically derived the parameters necessary to calculate a D-surface model that exactly reproduces the biological photonic structure. The lattice constant was determined to be 407 (± 11) nm and the volume fraction of cuticular material amounted to 35% (± 1.5%) in all inspected domains. Adjusting visualizations of the D-surface model to match the appearance of the photonic crystal in the exposed domains (Fig. 1b) provided the Miller indices of the exposed lattice planes. The corresponding normal directions of the lattice planes oriented parallel to the scale surface (see Fig. 3a, next page) are close to the <111> direction in yellow domains, the <100> direction in green and light blue domains and the <110> direction in dark blue

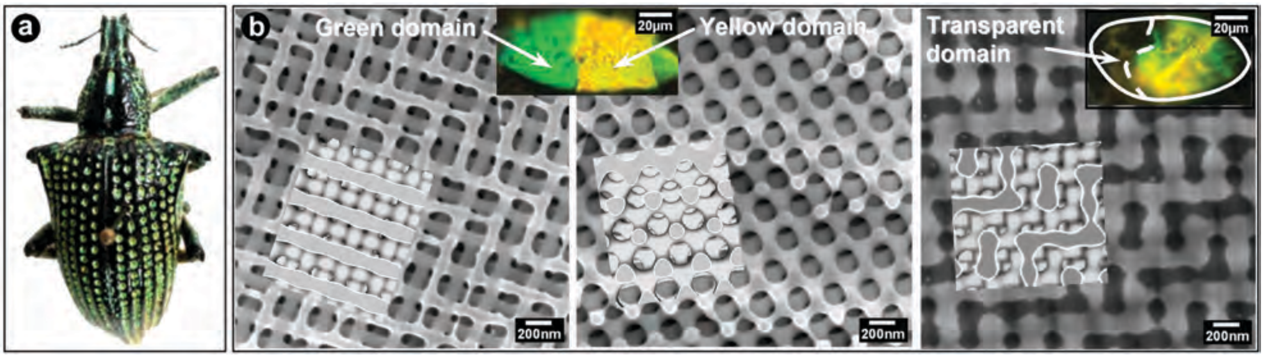

**Fig. 1:** *(a) The neotropic weevil Entimus imperialis (Coleoptera, Curculionidae). (b) Microstructure of the photonic crystal in coloured and transparent domains. The electron micrographs show the photonic crystal exposed parallel to the scale surface, the greyscale inserts corresponding visualizations of the D-surface model. The insert light micrographs show the exact probed locations on the respective scales.*

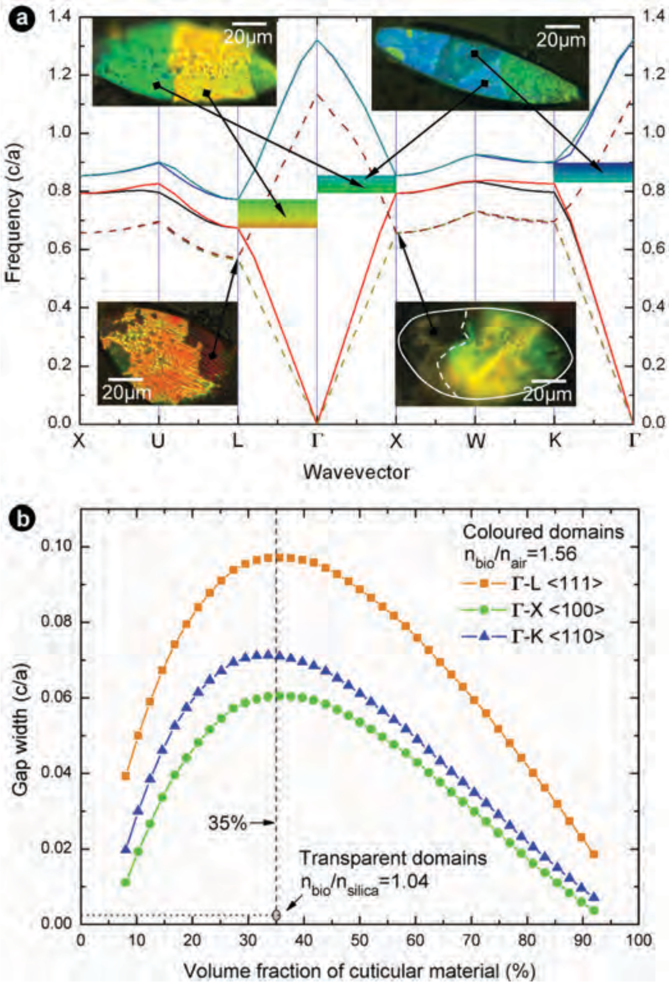

**Fig. 3:** *(a) Photonic band diagram for coloured and transparent domains. The probed locations (light micrographs) and the colour range of the band gaps (arrows) for the corresponding directions are shown as inserts. (b) Band gap width as a function of varying volume fractions of cuticular material. For three differently coloured domains, the band gaps obtain their widest frequency ranges at a volume fraction close to 35% (dashed line) as observed in the beetle. For transparent domains with low refractive index contrast, the band gaps are very narrow (circle).*

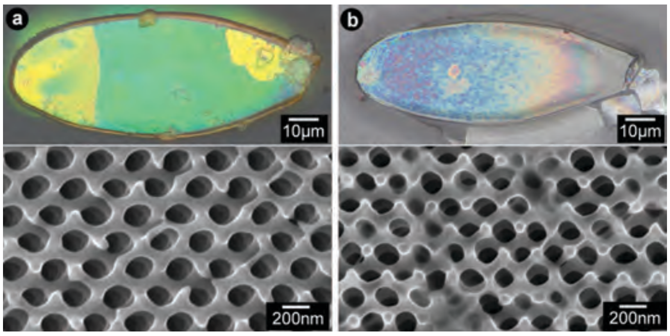

**Fig. 4:** *Comparision of appearance and microstructure of (a) a native scale and (b) its silica replica.*

domains. To validate the structural analysis of the photonic crystal in coloured and transparent domains of scales and compare their optical properties, we used the adjusted D-surface structure model to calculate the photonic band structure [5]. As refractive index of the cuticular network, we assumed 1.56 and we used 1.5 for the $SiO_2$ phase. The resulting photonic band diagram (Fig. 3a) shows partial band gaps in different directions. For coloured domains, the wavelength range of band gaps are 527-603 nm for Γ-L <111> (yellow domain), 476-513 nm for Γ-X <100> (green and light blue domains) and 453-492 nm for Γ-K <110> (dark blue domain) (see Fig. 3a). The observed colours in differently oriented domains and the wavelength ranges of the band gaps in the corresponding directions are in good agreement (Fig. 3a). By varying the volume fraction of the cuticular material from about 8% to 92%, the band gaps calculated for all investigated coloured domains obtain their widest frequency ranges when the volume fraction is close to 35 %, the value we determined for the beetle (Fig. 3b). Optically, a band gap covering a wider frequency range not only means more hues included, but also implies that a larger fraction of the incident white light is reflected. Thus, the scales show a stronger reflection and appear more brilliant.

In contrast, the combination of the $SiO_2$ phase and the cuticular phase in transparent domains shows only very narrow partial photonic band gaps due to the very small refractive index contrast between them (Fig. 3b). These narrow gaps only allow a very small fraction of the incident light to be reflected while the rest is transmitting through the scale. This weak reflection is sensitive to scattering. As a result, the domain appears transparent and dull to the eye.

Modification of the photonic band gap width, and thus the optical appearance, by replacing the air phase of a 3D photonic crystal with a second solid phase was observed for the first time in a beetle and offers great opportunities for the fabrication of tuneable biomimetic photonic crystals.

In collaboration with the group of Prof. Zollfrank (TU München), this biological photonic crystal has been biomimetically transferred into identical silica replicas with tuneable structural parameters [6] (Fig. 4).

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# Integrated Experimental-Numerical Analysis of Stress and Strain Partitioning in Multi-Phase Alloys

*C. Tasan, D. Yan, S. Zaefferer, E. Demir, D. Raabe,*
*M. Diehl, F. Roters, P. Eisenlohr, B. Svendsen, R. A. Lebensohn*

Department of Microstructure Physics and Alloy Design

Strain and stress partitioning is crucial in the behavior of multi-phase advanced high strength alloys, while its analysis is not possible using traditional experimental tools or by stand-alone numerical homogenization simulations. We therefore develop a novel integrated experimental-numerical methodology using experimentally obtained local deformation information to calibrate constitutive models for full-field crystal plasticity simulations.

The integrated methodology is as follows: Starting from large-area electron backscatter diffraction (EBSD) measurements conducted on a dual phase steel tensile test sample (Fig. 1a), representative microstructural regions are selected (Fig. 1b). The sample is imaged at increasing levels of strain (Fig. 1c) and local strains are measured using digital image correlation (DIC) (Fig. 1d). As final experimental step, orientation changes are measured using EBSD[1] (Fig. 1e). The simulations also start from the EBSD analysis of the undeformed microstructure, which is used to create the model (Fig. 1b). The initial crystallographic information of each point is taken directly from the EBSD measurement, and the distinction of martensite and ferrite is carried out based on the grain average image quality. The inset in Fig. 1f shows the resulting phase distribution. Both phases, martensite and ferrite, are modeled using a phenomenological crystal plasticity model [2] fitted to experimental stress-strain curves. The polycrystal stress-strain-curves for both phases are shown in Fig. 1f. The simulation is carried out using a spectral solver as described in [3] that is particularly suited for high mechanical phase contrast composites. These solvers make use of Fast Fourier Transforms (FFT) and are much more efficient than the FEM when simulating so called Representative Volume Elements. They, therefore, offer an unmatched resolution for direct full-field crystal plasticity simulations.

The experimental results presented in Fig. 2a (next page) reveal that: (i) the ferrite regions carry

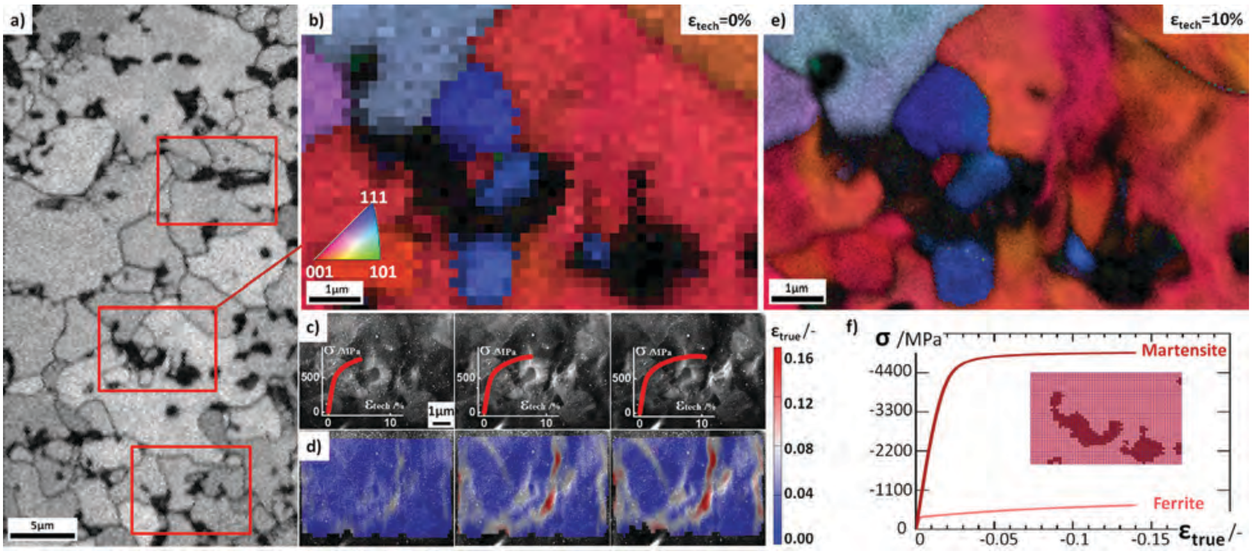

**Fig. 1:** *Experimental-Numerical Methodology:* ***(a)*** *Image quality (IQ) map obtained from a large area scan EBSD measurement,* ***(b)*** *Higher magnification IQ map of the selected region, with an inverse pole figure (IPF) overlay,* ***(c)*** *SE images, obtained during deformation in the horizontal direction, of the region shown in b (now covered by colloidal silica particles for DIC), with an overlay of the global stress and strain curve at the point of image acquisition,* ***(d)*** *local strain in the loading direction obtained from DIC analysis of the images shown in c,* ***(e)*** *IQ map and IPF overlay obtained from the area shown in b after deformation* ***(f)*** *Phase properties used in the numerical simulations, and an inset image showing the micromechanical model structure created from the EBSD measurement shown in b that serves as input to the full-field simulations.*

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[1] Note that both EBSD mappings can also be used to evaluate geometrically necessary dislocation densities from the calculation of the full dislocation density tensor [1].

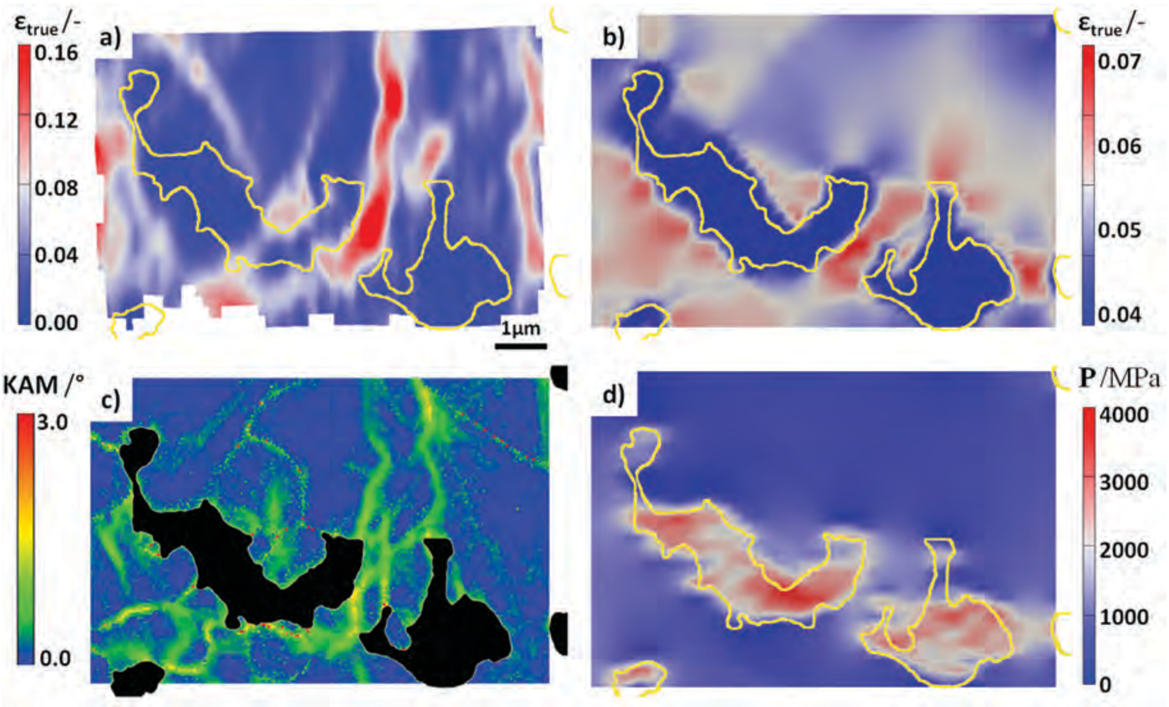

**Fig. 2:** *Experimental-numerical results of strain and stress distribution in the region shown in Fig 1b. Martensite islands are surrounded by a yellow line. (All strain and stress quantities are in the loading direction):* ***(a)*** *Local strain map obtained from DIC analysis,* ***(b)*** *Local strain map obtained from numerical simulation,* ***(c)*** *kernel average misorientation map obtained from EBSD data,* ***(d)*** *Local stress map obtained from numerical simulation.*

most of the strain while the martensite remains nearly undeformed; (ii) the strain distribution in the ferrite is very inhomogeneous. This micromechanical heterogeneity is confirmed by the kernel average misorientation map presented in Fig. 2c, showing a similar distribution for the local misorientation. The locations of the high-strain bands with respect to the martensite islands suggest that the martensite phase dispersion and morphology governs strain localization. More specifically, strain localization effects occur in regions where bulky martensite islands are separated by a narrow gap of ferrite in-between and where irregularities in martensite geometry cause local stress peaks.

The strain distributions obtained from the full-field crystal plasticity simulations (Fig. 2b) show good qualitative agreement with those obtained from experiments (mind the different scales in Fig. 2a and b) reproducing the majority of the deformation bands. Quantitatively however, the simulations reveal less pronounced strain partitioning, suggesting that the single phase properties used are not exactly matching those of the real constituents.

The stress distribution obtained from the simulations (Fig. 2d) shows that most of the stress in the material is carried by the martensite phase. More importantly, the detrimental effect of irregularities in the martensite morphology is also underlined: Highest stresses occur in the narrow regions of the martensite islands. This correlates well with earlier observations showing that martensite sphericity plays an important role for its plastic deformation limits [4].

To conclude, a novel joint experimental-numerical micromechanical methodology is being developed that allows analyses of strain and stress partitioning in complex multi-phase materials. The preliminary results show a promising correlation between the experiments and corresponding full-field crystal plasticity FFT simulations. The results demonstrate the importance of martensite dispersion and sphericity in dual phase steels for the integral mechanical behavior. Current emphasis is placed on improving the quality of the simulations further by feeding in more realistic phase properties for ferrite and martensite.

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# Paramagnetic Phonons and Free Energies from *ab initio*: A First-Principles Prediction of the Anti-Invar Effect in fcc Fe

*F. Körmann, B. Grabowski, B. Dutta, T. Hickel, J. Neugebauer*

Department of Computational Materials Design

Dynamic processes on the atomic scale determine the kinetics and thermodynamics of steels. Such processes are behind many technologically relevant mechanisms, but are often only poorly understood. An example is the anti-Invar effect in fcc Fe, i.e., a large and constant expansion coefficient for a wide temperature range. For theoretically describing the free energy of such mechanisms, the simulation of the dynamics is critical. These calculations require the computation of the forces acting on individual atoms. In the case of magnetic materials, however, the reduction of magnetic order makes current *ab initio* approaches often not suited for describing forces at finite magnetic temperatures. Using ordered magnetic states instead is for the chosen example fcc Fe not an option, since they yield dynamic instabilities.

Within in the last few years, several approaches based on dynamical mean field theory, non-collinear spin-spiral calculations, or spin MD were proposed to overcome this limitation. They have in common that they are not only computationally expensive, but also inhibit a conceptually increased level of complexity. As a consequence the prediction of thermodynamic properties of paramagnetic materials at finite temperatures such as linear expansion coefficients or bulk modulus has not been achieved so far.

We recently introduced a scheme to compute atomic forces at finite magnetic temperatures, for which we developed a spin-space averaging (SSA) procedure [1]. In the proposed scheme the SSA forces are obtained by coarse-graining the magnetic configuration space. For example, the atomic forces in the high-temperature paramagnetic state, where the local magnetic moments are randomly distributed over the lattice, are obtained by statistical averaging over a sufficiently large set of magnetic structures, as sketched in Fig. 1. In practice the magnetic configurations are constructed using the concept of special quasi-random structures as obtained from the ATAT package.[1] The computational efficiency can be further improved by employing in addition the underlying crystal symmetries [1].

From the effective SSA forces the phonon spectra can straightforwardly be deduced. In Fig. 2 we demonstrate that the theoretical results of our new

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[1] To simplify the modeling of the PM state we consider here collinearly disordered magnetic moments only. The proposed scheme itself is, however, very general and would, in principle, allow the incorporation of non-collinear structures.

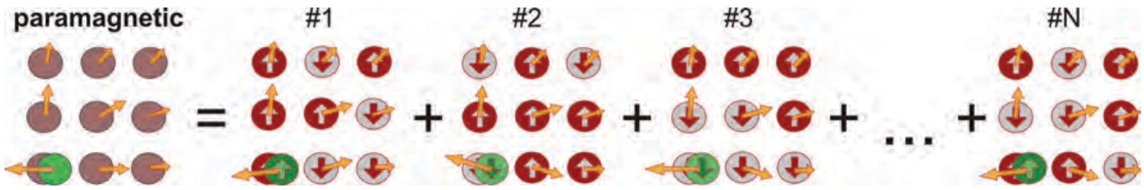

**Fig. 1:** *Sketch of the SSA procedure. The effective forces at finite magnetic temperatures are obtained from a set of disordered magnetic configurations.*

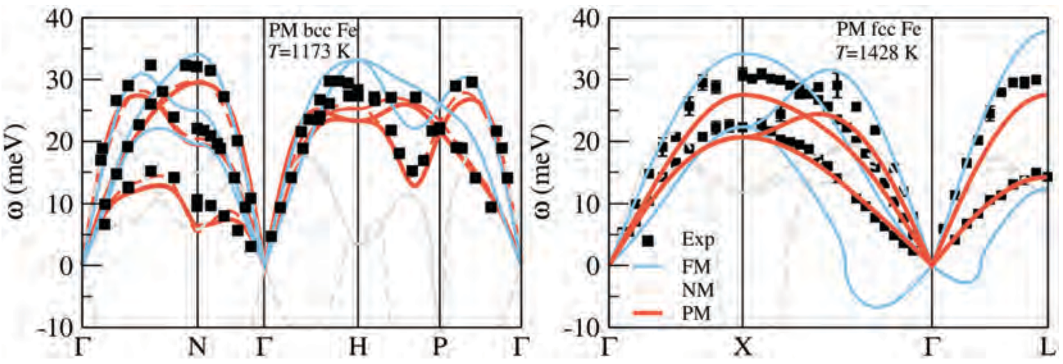

**Fig. 2:** *Phonon spectra of bcc and fcc Fe above the magnetic ordering temperatures. Computing the spectra with the SSA scheme to describe paramagnetism (PM) provides excellent agreement with experimental data in contrast to ferro- (FM) or non-magnetic (NM) calculations.*

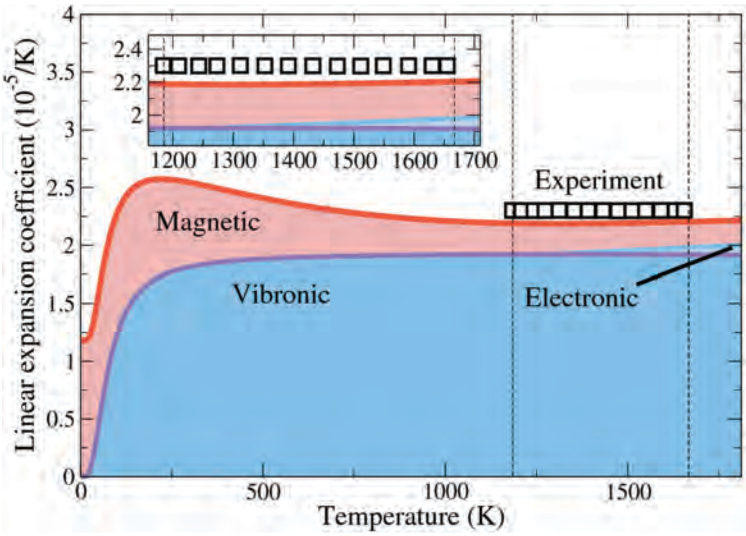

**Fig. 3**: *Comparison of the theoretical linear expansion coefficient for fcc Fe (red line) with experiment (black symbols [4]). The dashed vertical lines indicate the stability regime of fcc Fe. The inset provides a zoom-in into the fcc stability regime.*

scheme for bcc and fcc Fe agree very well with experimental data in the paramagnetic (PM) state. Even particularities such as the strong phonon softening for bcc Fe around the N-point (reflecting the infamous strong decrease in the $C'$ and $C_{11}$ elastic constants at higher temperatures) are reproduced. Furthermore, the dynamical instability of non-magnetic bcc Fe at 1173 K is lost in the PM state. For the present discussion more decisive is the fact that also in case of fcc Fe the magnetic disorder is sufficient to remove the dynamic instabilities, being present in ferro-/nonmagnetic calculations.

We can make further use of the clear advantages of the SSA scheme that it can be easily extended to compute vibronic free energy contributions with already existing statistical concepts such as, e.g., the quasi-harmonic approximation. Combining the SSA scheme for the vibronic entropy with explicit electronic and magnetic contributions [2] enables us to compute a completely *ab initio* derived free energy surface for fcc Fe. Only in this way it is now possible, to determine the linear expansion coefficient for fcc Fe. The comparison with available experimental data in Fig. 3 yields an excellent agreement. Within the new scheme it is even possible to reproduce and understand the (long debated) anti-Invar effect in fcc Fe [3]. As can be seen from Fig. 3 the source of the high and constant expansion coefficient is mainly due to vibronic contributions revealing the significant impact of the volume dependence of paramagnetic lattice vibrations/phonons.

In summary, we have extended our previous methods [2] to account for the delicate interplay between atomic and magnetic degrees of freedom at high temperatures. The developed SSA procedure provides not only an excellent scheme to compute atomic forces at finite magnetic temperatures, but allows further, in combination with statistical concepts, the computation of free energy surfaces in the paramagnetic regime.

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# Dual Scale Modeling of Phase Equilibria

*D. Korbmacher* [1], *R. Spatschek* [1], *J. von Pezold* [1], *C. Hüter* [1],
*J. Neugebauer* [1], *S. Brinckmann* [2]

[1] Department of Computational Materials Design
[2] ICAMS, Ruhr-Universität-Bochum

The basis for a theory guided design of new steels and other novel materials with superior properties is the development of a multiscale simulation chain, which transfers information from one lengthscale to the next. This is absolutely necessary also for understanding phenomena like hydrogen embrittlement [1] and other material failure mechanisms, as well as the finding of new battery materials [2]. It comprises the scale-bridging modeling of phase equilibria and transitions in complex materials, ranging from macroscopic dimensions down to the nanoscale. For this, an efficient and accurate matching between the atomistic simulations and formal thermodynamic and continuum concepts is critical. We have therefore studied approaches that seamlessly connect the atomistic and continuum scale, illustrated for the Ni−H system. Our approach provides important fundamental insights into the theory of phase equilibria in coherent solid-state systems such as nanodispersion strengthened or electrical steels, as it elucidates quantitatively the role of different energetic and entropic contributions.

The starting point of our study is the determination of the equilibrium spatial distribution of the interstitial H atoms in the metallic matrix, employing Monte-Carlo simulations and molecular statics. Depending on the H chemical potential dilute or condensed H distributions are obtained. The condensed hydride precipitates remain coherent and adopt characteristic shapes depending on the bulk H concentration, as shown in Fig. 1. The chemical potential of the hydrogen atoms, $\mu_H$, as a function of the average concentration deviates significantly from its expected functional form based on the common tangent or Maxwell construction.

Our starting point for transferring this complex atomic scale behavior to the continuum level is the free energy for the single phase material, $F = F_{el} + \mu_0 N_H + F_c + F_{H\text{-}H}$, with the number of hydrogen atoms $N_H$ and the elastic free energy $F_{el}$, the configurational free energy $F_c$ and the hydrogen-hydrogen interaction $F_{H\text{-}H}$. $\mu_0$ is the solvation energy needed to insert an isolated hydrogen atom into the (empty) matrix. The hydrogen-hydrogen interaction reflects the lattice mediated attraction between hydrogen atoms, which are dissolved in the matrix. The configurational contribution stems from the different combinatorial possibilities to occupy the octahedral sites with hydrogen. Together, they constitute the typical “van-der-Waals loop” (green curve in Fig. 1).

Phase coexistence on this level is described by Maxwell's equal area rule, which states that phase separation sets in at the intersection points of a horizontal line with the S-shaped van der Waals loop, cutting it into two equal areas above and below this Maxwell line (blue line).Obviously, at this level

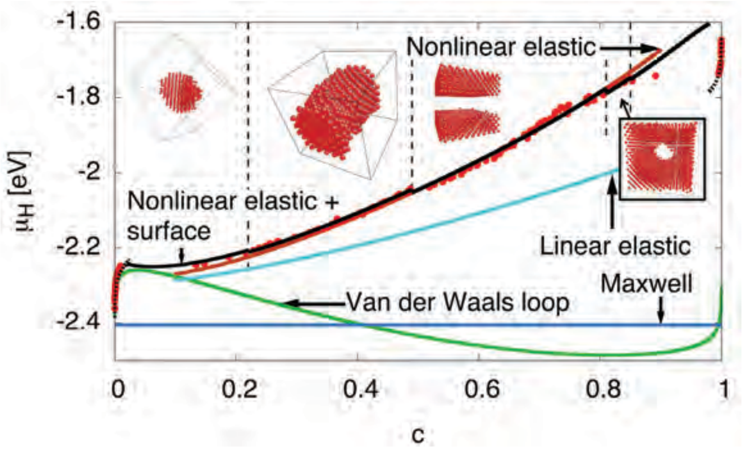

**Fig. 1:** *The chemical potential of hydrogen at T = 300 K. The red dots are the data from the Monte Carlo simulations, the green curve is the calculated van der Waals curve. Phase equilibrium without elastic and interfacial effects represented by the blue horizontal Maxwell line. Modifications due to cubic linear elasticity are given by the cyan curve. The chemical potential including nonlinear elastic effects (brown) is very close to the atomistic data, and together with interfacial effects (black) the agreement is even more convincing. The insets show the different concentration dependent patterns, the vertical dashed lines separating the concentration regimes.*

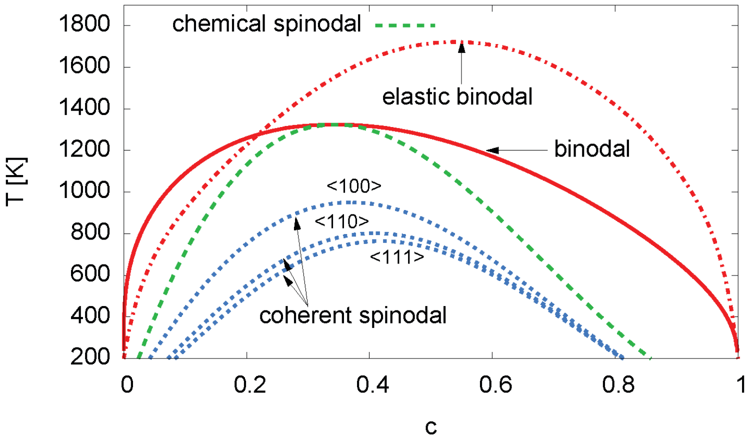

**Fig. 2:** *Phase diagram and spinodals of the Ni-H systems, based on parameters extracted from Monte Carlo simulations. The concentration is 1 if all octahedral sites are filled, i.e. equal number of Ni and H atoms. The solid red line is the binodal without consideration of elastic effects, whereas the dash-dotted line is the same with elastic effects for fixed volume. The chemical spinodal (green) ignores elastic effects and touches the binodal at the critical point, whereas the coherent spinodals (blue) take into account deformations for density variations in the given directions. Spinodal decomposition is possible below the curves.*

the agreement with the fixed volume atomistic data is not good at all. The large deviations between the atomistic data and the continuum model clearly indicate that elastic and interface effects are critical and cannot be neglected. The pure nickel and the hydride exhibit a substantial lattice mismatch, leading to the cyan curve shown in Fig. 1. Since we still observe a significant discrepancy to the Monte Carlo data, we therefore conclude that the consideration of linear elasticity is not sufficient to explain the slope of the chemical potential in the two phase region.

The reason for this discrepancy is the appearance of large compressive stresses for higher hydrogen concentrations implying that nonlinear elastic effects have to be taken into account. With them the continuum chemical potential shows now a much more satisfactory agreement with the Monte Carlo data (see the brown line in Fig. 1).

In a final step we take into account interfacial effects. Although they give only a small contribution, they determine the shape of the precipitates. For low concentrations we expect spherical hydride inclusions, followed by tubular and slab-like precipitates. For high concentrations, when instead the nickel phase nucleates inside the hydride, the arrangement is similar. In our atomistic calculations we indeed find all these structures in the correct ordering (see Fig. 1).

Including all energy contributions we are able to successfully transfer the atomistic onto the continuum scale. This allows us e.g. to predict the entire bulk phase diagram without and with elastic effects, see Fig. 2. We see the tremendous influence the elastic effects have on phase stability, with an enlargement of the two-phase region towards higher temperatures and the hydrogen rich side. This unusual reduction in solubility - one would intuitively expect the suppression of phase separation since coherency stresses are energetically unfavorable - is due to deviations from Vegard's law.

Finally, our approach allows to predict the onset of spinodal decomposition, going beyond the purely static equilibrium concepts considered so far. In the spinodal regime the homogeneous mixture is unstable, whereas in the remaining two-phase region phase separation is initiated by nucleation processes, requiring an activation energy. Spinodal decomposition is suppressed since density fluctuations provoke elastic stresses, leading to the coherent spinodal regime, as shown in Fig. 2 for density variations in different lattice directions.

Altogether, the determination of phase diagrams nicely demonstrates the opportunities arising from the transfer of atomistic data to the mesoscale: We point out that the results shown in Fig. 2 are practically impossible to obtain accurately using atomistic simulations only, as this requires the modeling of very large systems and the clear distinction from nucleation events for the spinodal decomposition. The resulting description can then also directly be used in mesoscale simulations models like phase field.

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# Extending *ab initio* Simulations of Point Defects up to the Melting Temperature

*A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer*

Department of Computational Materials Design

Many technologically relevant processes are ultimately connected to point defects. Prominent examples are thermodynamic phase stabilities governing phase transformations or diffusion processes determining the concentration profile and segregation kinetics. Point defects have also a strong impact on mechanical strength and ductility of structural materials by acting as pinning centers for dislocations or by enabling dislocation climb.

The natural quantity to characterize point defects is their Gibbs energy of formation, $G^f(T) = H^f(T) - TS^f(T)$. An experimental determination of the temperature dependence faces great difficulties as only a small high-temperature window is directly accessible (see Figs. 1 and 2). Differential dilatometry (DD), on the one hand, yields in the case of Cu from the melting point of 1360 K down to about 1200 K a smooth curve of data points. Below 1200 K, however, the scatter in the data indicates that the statistics is too poor to sufficiently resolve the vacancy related differences between an increase in the macroscopic length and in the lattice constant. Positron annihilation spectroscopy (PAS), on the other hand, allows one to assess a slightly lower concentration window, but is unable to resolve concentrations above $10^{-4}$ as saturation effects set in prohibiting accurate measurements.

For describing $G^f(T)$ it is therefore common practice to assume simplifying (i.e., Arrhenius like) temperature dependencies, $G^f = H^f - TS^f$, with constant $H^f$ and $S^f$ fitted to available high temperature data. However, these results show often only poor agreement with *ab initio* formation enthalpies of $H^f$, determined at T = 0 K, even for 'simple' elements like Cu or Al. As an additional complication, already small scatter in the high-temperature experimental data yields in the extrapolations over wide temperature ranges large uncertainties in the extrapolated $H^f$ at $T = 0$ K. Finally, $G^f$ seems to show for DD and PAS qualitatively different temperature dependencies. Two scenarios have been discussed in the literature to explain these inconsistencies. Scenario (A) assumes that $G^f$ is non-linear with a temperature dependent $H^f(T)$ and $S^f(T)$. Alternatively, the change in concentration is explained in scenario (B) by a

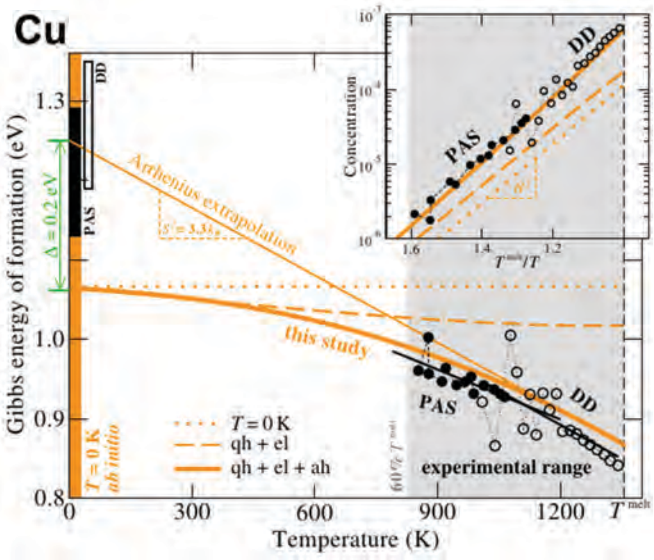

**Fig. 1:** *Experimental (black symbols, lines, and stripes) and ab initio (orange lines) vacancy formation energies in bulk-Cu. Experiments (PAS=positron annihilation spectroscopy [6], DD=differential dilatometry [7]) are limited to temperatures close to the melting point (gray shaded region). Extrapolations of DD and PAS data introduce uncertainties (filled and empty black stripes in upper left corner) hampering comparison with T = 0 K ab initio data. The present DFT study closes the gap between experiment and theory (bold solid orange line).*

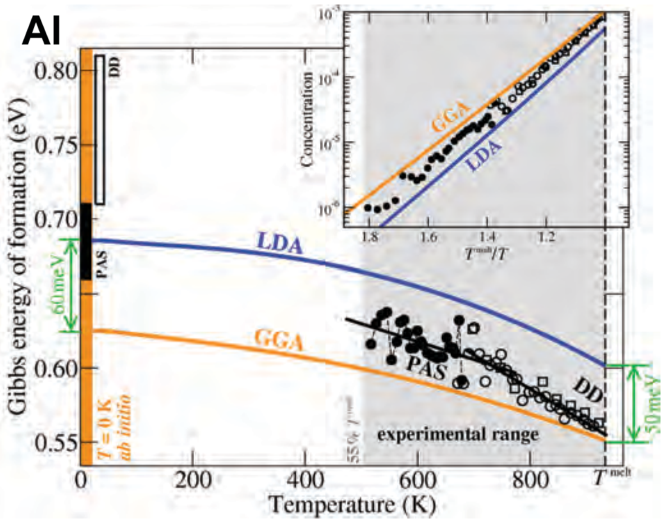

**Fig. 2:** *Possibilities and limitations of the two most popular DFT exchange-correlation functionals, LDA and GGA. The example shows the properties of monovacancies in Al. While showing an almost constant shift (originating from differences in the T = 0 K results), the clearly non-linear temperature dependence is well described by both functionals. Experimental data are from Refs. [6] (●), [8] (□), and [6] (○).*

superposition of mono- and divacancies, the latter dominating the slope of $G^f$ at high temperatures [1].

In order to resolve this long standing debate, we have performed highly accurate temperature-dependent DFT simulations of mono- and divacancies in Al and Cu [2]. We apply our previously developed techniques to include a complete description of electronic and ionic finite temperature excitation mechanisms as well as their thermodynamic coupling. The often used simplifying assumption of non-interacting phonons is dropped: Phonon-phonon interactions are considered accurately yet efficiently by lattice dynamics employing our recently developed hierarchical coarse graining scheme. This scheme achieves a reduction from $10^7$ configurations usually necessary to sample the configuration space to only $10^2$ configurations at full *ab initio* accuracy [3].

Based on our calculations we can rule out that divacancies are the reason for the non-Arrhenius behaviour for Al and Cu as assumed in literature (scenario B). At $T$ = 0 K, we find the divacancy to have only a small binding energy (~80 meV in the case of Cu). The small energy indicates that the divacancy dissociates into two isolated vacancies for high temperatures and characteristic concentrations. An even stronger argument to discard the divacancy is related to the slope of $G^f$ at finite temperatures. In order to explain the difference between DD and PAS within the mono-divacancy scenario (B), a significantly larger $S^f$ for divacancies has to be assumed. Our results disprove this assumption: The *ab initio* computed entropy of formation is very similar in magnitude for di- and monovacancies. As a consequence, the divacancy concentration is even at the melting temperature negligible ($10^{-7}$) for both Al and Cu with respect to the monovacancy concentration ($10^{-3}$).

We can therefore conclude that deviations from a linear (Arrhenius) behaviour of the monovacancy $G^f$ are responsible for the experimental observations. Being able to compute all free energy contributions allows us to systematically check the agreement with the various levels of theory. The dotted line in Fig. 1 shows the $T$ = 0 K *ab initio* value which, as mentioned earlier, does not agree with the value extrapolated from experiment. The dashed line additionally includes the influence of non-interacting but volume dependent phonons (quasiharmonic approximation) and it is clear that a significant discrepancy with experiment remains. The vanishing slope at high temperatures resembles vanishing entropy ($S$ ~ 0.0 $k_B$). Electronic entropy effects are found to be negligible at this scale. Adding finally explicit anharmonic contributions (bold solid orange line) an excellent agreement with experiment is found. In particular, the curvature of the Gibbs formation energy accurately captures the deviating slopes of PAS and DD data.

Having this formalism we systematically checked the performance of the various exchange-correlation (xc) functionals. Fig. 2 shows the results of such calculations for Al vacancies and the two most commonly employed functionals, the local-density (LDA) and the generalized gradient approximation (GGA). The two functionals bound the experimental data, a behaviour we consistently find also for other elements [4]. We further observe that the *ab initio* temperature dependence follows the experimental results remarkably close. Both observations further substantiate our earlier findings [5] that (i) DFT based thermodynamic properties are mainly limited by the accuracy at $T$ = 0 K and that (ii) the comparison of several xc-functionals can provide a confidence interval for the accuracy of the *ab initio* results.

In conclusion, the almost universally applied assumption of temperature independent $H^f$ and $S^f$ (linear Arrhenius behavior) is not justified when extrapolating high-temperature data to T = 0 K. Using the correct temperature dependence, which was unknown before this study, we find corrections in the order of a few tenth of an eV for the vacancy formation energies and an order of magnitude for the entropies. The new formalism allows us to compute finite temperature point defect energies with hitherto unprecedented accuracy – being important for realistic applications as well as for improving the predictive power of DFT calculations, where these energies are often used as benchmarks.

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# Strong and Weak Magnetic Coupling in Chromium

*F. Körmann*[1], *B. Grabowski*[1], *M. Palumbo*[2], *S.G. Fries*[2], *T. Hickel*[1], *J. Neugebauer*[1]

[1] Department of Computational Materials Design, [2] ICAMS, Ruhr-Universität Bochum

Chromium is a key material in many practical applications and, in particular, a decisive ingredient for stainless steels. At low temperatures bcc Cr displays antiferromagnetic order in form of an incommensurate spin density wave (SDW), which disappears at a critical (Néel) temperature of $T_N$ = 311 K. While this temperature regime is well understood today, several observed anomalies in the high-temperature thermodynamic properties of Cr leave many questions open [1]. We have collected results of various measurements from the last thirty years (literature research at ICAMS), which revealed peculiarities in the expansion, its coefficient, heat capacity and elastic moduli well above the Néel temperature (black symbols in Fig. 1). One example is the enormous increase in the linear expansion coefficient (Fig. 1b). It even strongly exceeds the ones of Mo and W, which are themselves known to have high coefficients due to anharmonic contributions. In the case of Cr, it was speculated that again anharmonic or alternatively magnetic contributions are responsible for the strong increase in the thermodynamic data [2]. In particular the latter attracted a lot of interest [1]. Due to the comparable low $T_N$, many theoretical approaches including well-established CALPHAD databases, assume rather weak magnetic contributions. On the other hand, several works provided indications for strong magnetic contributions (see e.g. [1]).

In order to clarify the role of the different contributions we performed state-of-the-art first-principles techniques including *ab initio* molecular dynamic simulations [3] and spin quantum Monte Carlo simulations [4] to treat the explicitly anharmonic lattice vibrations and magnetic free energies. Using our previously developed methodology [4,5], we parameterize an effective nearest-neighbor Heisenberg Hamiltonian by tuning the exchange

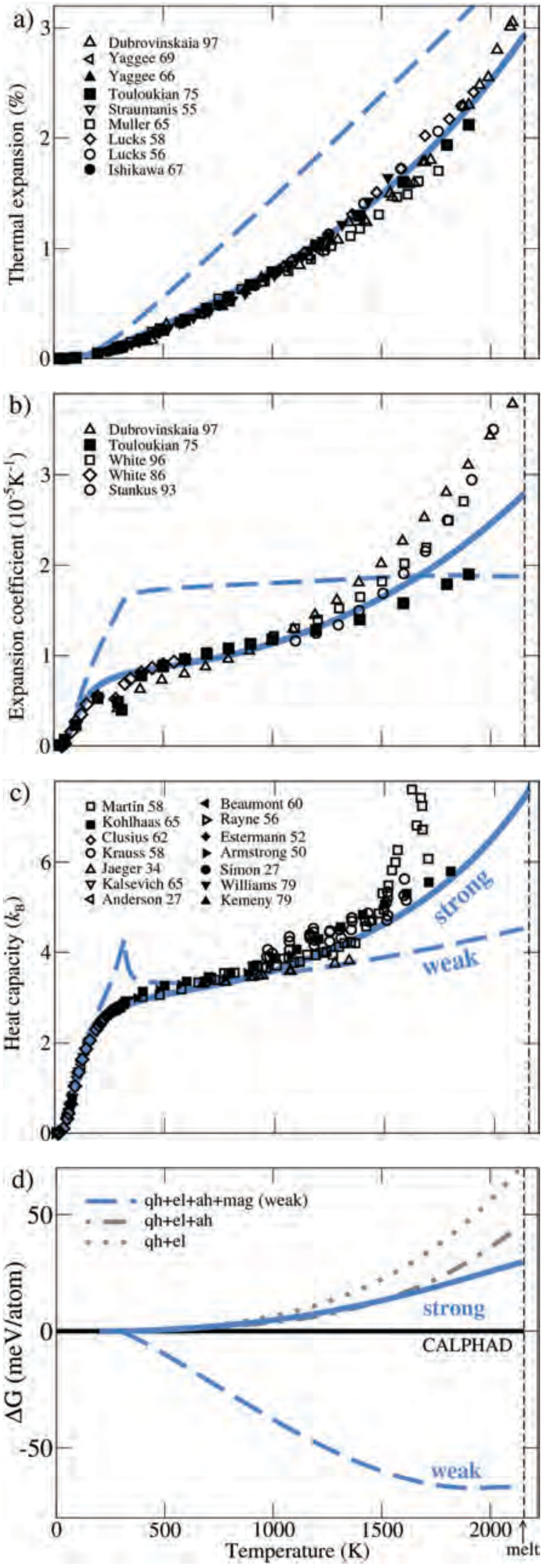

**Fig. 1:** *Temperature dependence of thermodynamic properties for bcc Cr: a) linear expansion, b) linear expansion coefficient, c) heat capacity, and d) Gibbs energy. Black symbols are experimental values and blue lines show our theoretical results. The dashed (solid) line corresponds to the weak (strong) coupling scenario. Vertical dashed lines indicate the melting point (2156 K). The Gibbs energy in d) is referenced with respect to values obtained from the CALPHAD approach (SGTE unary database). Additionally the dependence of the quasiharmonic and electronic (qh+el) contribution and the one of the quasiharmonic, electronic and anharmonic (qh+el+ah) contribution are shown.*

interaction to reproduce the experimental $T_N$ = 311 K. The quasiharmonic and electronic free energy contributions have been obtained with two different DFT codes (VASP and Quantum Espresso) and yield consistent results. The anharmonic excitations have been computed for more than 30 volume-temperature points to systematically check this contribution over the full temperature range. The resulting thermodynamic properties are shown by the dashed lines in Fig. 1 and compared to the experimental data. The comparison reveals clear and consistently large deviations for all thermodynamic properties. Based on our analysis we conclude that, despite the low $T_N$, the picture of a weak magnetic coupling scenario in Cr is incorrect.

In fact, a number of experimental and theoretical approaches indicate that huge magnetic spin fluctuations may be present in Cr even well above $T_N$. As recently discussed by Jaramillo and coworkers, the origin is related to the intrinsic coupling of the SDW to a charge density wave [6]. Based on the involved electron-hole pseudo gaps shown by optical measurements, it was concluded that high energy excitations on an energy scale of ~$5k_BT_N$ are present in Cr. This coupling between charge and spin density waves can result in strong magnetic fluctuations. Jaramillo and co-workers provided an estimate of the magnetic exchange interaction of 140 meV, much larger than one would expect from $T_N$ = 311 K (26.8 meV). Further, there are several experimental studies addressing the magnetic degrees of freedom directly. These studies indicate that Cr exhibits strong magnetic coupling effects: Spin wave excitations with energies up to 400 meV and spin wave velocities up to $1.5\times10^5$ m/s were found in $Cr_{0.95}V_{0.05}$ samples [7]. Neutron scattering experiments suggest strong magnetic interactions at least up to 600 K. Magnetic correlations were observed that extend over 11 bcc unit cells even at 700 K, i.e., temperatures well above the Néel temperature [1,8]. A general conclusion of all these studies is that the phase above $T_N$ remains a highly correlated regime.

To clarify if a strong magnetic coupling provides an explanation for the observed anomalies in the thermodynamic properties, we pursued the following scenario [9]: The observed strong magnetic fluctuations are mimicked by assuming a large spin-interaction parameter in our magnetic model. More precisely the solid blue lines in Fig. 1 correspond to a value of 100 meV as compared to the 26.8 meV belonging to the weak-coupling scenario (dashed lines). Note that all plotted dependencies for the resulting thermodynamic quantities, include again electronic, quasiharmonic, and anharmonic contributions.

The strong-coupling scenario provides a consistently good description over the whole temperature range for all thermodynamic quantities. This consistent description of materials properties is remarkable keeping in mind that the different thermodynamic observables explore rather different paths and derivatives on the complex free energy surface.

From these results we can conclude that the temperatures at which one can expect a magnetically fully disordered state are considerably higher than $T_N$. Furthermore, anharmonic contributions beyond the quasi-harmonic approximation are not the dominant source for the unusual thermodynamic behavior at higher temperatures. The excellent agreement with experiment up to the melting point implies that the temperature-dependent magnetic effects of bcc Cr can be accurately approximated by an effective Heisenberg Hamiltonian with strong magnetic coupling. The value of 100 meV identified here by a thermodynamic analysis is in striking agreement with a recent estimation of Jaramillo and coworkers [6], which probe the spin and charge order parameters using X-ray diffraction.

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# Dangling-Bond Defects in Amorphous Materials

*G. Pfanner, C. Freysoldt, J. Neugebauer*

Department of Computational Materials Design

Defects crucially modify the electrical, optical, mechanical, and other properties of real materials. Whenever a material is processed, defects may be created or transformed. Theoretical insights into the relevant mechanisms promise to improve or even open completely new processing routes, and is therefore of great practical interest for innovation. On the atomistic scale, defects can be regarded as imperfections in the ideal crystalline order. Viable methods are nowadays available to calculate the relevant properties of such defects with highly accurate electronic-structure methods, notably density-functional theory [1]. But what if an ideal crystalline order does not exist because the material is amorphous? How can we then characterize a defect?

This conceptual question has been a guiding motif in the BMBF-funded EPR-Solar project on the dangling-bond defect in hydrogenated amorphous silicon (a-Si:H) during the past five years. a-Si:H has the largest market share in thin-film solar cells. Such thin film cells offer advantages in raw material use, production cost, availability of raw materials, and handling. The major drawback of a-Si:H-based solar cells is their limited efficiency, which is related to the inherent presence of dangling-bond (db) defects, i.e., singly undercoordinated silicon atoms. Unfortunately, the dangling-bond concentration is further enhanced by illumination (Staebler-Wronski effect), leading to a 30% relative loss in efficiency in the early lifetime of the solar cell [2].

Dangling bonds can be experimentally observed by electron paramagnetic resonance (EPR) as they contain in their neutral state an unpaired electron which aligns either parallel or anti-parallel in an externally applied magnetic field. In EPR, transitions between the corresponding energy levels are induced by microwave radiation. In the case of a-Si:H, EPR indicated a close connection of the db defect to the Staebler-Wronski effect. Despite tremendous research efforts in the past 40 years, it is still not fully understood and can be suppressed only in part. In the EPR-Solar project, leading experimental groups in EPR spectroscopy from Berlin, Munich, and Jülich joined up with the CM department of the MPIE to (figurally) shed more light on the dangling-bond defect in a-Si:H by a combination of advanced EPR measurements (multifrequency analysis, sub-μm spatial resolution, time-resolved spectroscopy) and theoretical modelling.

The EPR signal of the dangling bond consists of a broad feature corresponding to a Zeeman splitting g = 2.0055. At low magnetic fields (and thus low microwave frequencies), hyperfine satellites from the coupling to the central $^{29}$Si isotope (5% natural abundance) become visible, with an average hyperfine coupling of ~180 MHz. This hyperfine coupling turns out to be 40% lower than dangling-bond-like defects in crystalline silicon (c-Si), e.g. at a Si/SiO$_2$ interface or in vacancy-impurity complexes. The full powder spectrum at different frequencies can be calculated from a model spin Hamiltonian

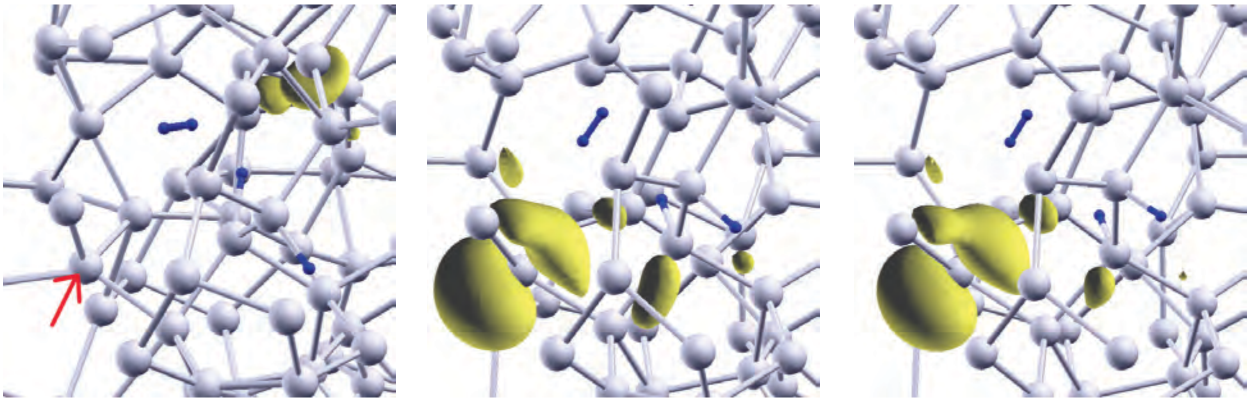

**Fig. 1:** *Spin density (yellow) of a dangling-bond system in a-Si:H (grey: Si, blue: H) for different strain states: -7%, 0%, and +8%. For strong compressive strain (left), the spin is no longer associated with the previously undercoordinated atom (red arrow). For tensile strain, the spin becomes more localized (right).*

with Gauss-broadened g- and hyperfine (A-) tensors. Conversely, by fitting the simulated spectrum to experiment, the hyperfine and Zeeman tensors can be extracted. The experiments carried out within the EPR Solar project revealed that the A-tensor shows an axial symmetry, whereas the g-tensor has three independent components, the lowest one being close to the g-value of the free electron (2.0023) [2].

We approached the problem of interpreting these experimental findings from two sides: first a systematic study of structure-property relationships in well-defined periodic model systems (some of them even known experimentally), and, second, by a statistical analysis of a defect ensemble in models of the amorphous structures. For the latter, defects were created at random positions in the network by abstracting a hydrogen atom from the defect-free model. The systematic study confirmed the well-known notion that the isotropic (Fermi contact) and anisotropic (dipolar) hyperfine couplings are mostly determined by the bonding geometry at the three-fold coordinated db atom: flat geometries lead to a dominant p-character of the dangling-bond orbital which contributes to the anisotropic, but (for symmetry reasons) not directly to the isotropic coupling. Tetrahedral geometries, on the other hand, admix an s-character and show larger isotropic, but lower anisotropic coupling. However, this effect is strongly overlaid by the effect of delocalization away from the central atom [3], which could not be observed in older cluster calculations. In c-Si, the delocalization correlates with the geometry since the orbital character determines the energetic position within the band gap (additionally altered by nearby impurities), and the energetic proximity to the valence band leads to a delocalized defect state. The g-tensor, on the other hand, is only weakly modified by geometrical variations and stays almost perfectly axial in all considered c-Si systems.

These fundamental mechanisms are also active in the amorphous matrix, but their relative importance varies depending on the specific surroundings of the defect. Surprisingly, delocalization is more important in the amorphous state despite the larger band gap and larger effective masses of the bulk material: apparently, the distorted geometries foster an electronic coupling to nearby fully coordinated atoms. These geometric distortions also explain the loss of symmetry in the g-tensor: in contrast to the hyperfine coupling, which is exclusively determined by the spin density and hence the orbital character at the dangling-bond atom, the g-tensor beyond the free-electron value ($\Delta g$) arises from induced spin currents, which sensitively react to disorder in bond lengths and bond angles. Quantitatively, our defect ensemble reproduces well the peak values of the g-tensor distributions, with some overestimation of the variance [4]. For the hyperfine tensor, we demonstrated that the delocalization explains in part the experimentally observed red-shift. The remaining discrepancy is most likely due to a somewhat oversimplified selection of the theoretical defect ensemble: in experiment, defects will not appear at random positions, but will be filtered by thermodynamic equilibration and kinetic effects in the creation and diffusion. A broad analysis of various aspects of the amorphous model systems underpinned our conclusion that the dangling-bond defect in a-Si:H is a 'network defect' that cannot be conceptually separated from its immediate surrounding [5]. Its electronic, geometric, and spectroscopic characteristics sensitively react on variations in the environment as e.g. induced by strain (see Fig. 1). Dangling bonds can even merge into the network under moderate compressive strain, developing a floating-bond-type (overcoordinated) defect by forming a new bond.

Our strategy of combining a systematic analysis to discover fundamental mechanisms with a statistical modelling of a representative ensemble to capture the natural variability of disordered systems can be applied also to other cases. For instance, corrosion products of structural materials (transition metals) are typically off-stoichiometric, disordered, and sometimes even amorphous compounds consisting of cations in different oxidation states, and oxide and hydroxide anions (not to talk about anion vacancies). The ion transport across these films determines critically the speed of on-going corrosion, and it is ultimately linked to the diffusion of point defects. Therefore, disordered oxides will be addressed within an upcoming DFG Forschergruppe (in preparation).

**References**

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4. Pfanner, G.; Freysoldt, C.; Neugebauer, J.: Phys. Rev. B 83 (2011) 144110.
5. Pfanner, G.: “The dangling-bond defect in silicon. Insights into electronic and structural effects from first-principles calculations of the EPR parameters“, PhD thesis, Universität Paderborn (2012). Also: Pfanner, G.; Freysoldt, C.; Neugebauer, J.; Jarolimek, K.; Inam, F.; Drabold, D.: *to be submitted*.

## PART IV.

# GENERAL INFORMATION AND STATISTICS

# Boards, Directors, Max Planck Fellows, External Scientific Members and Guest Scientists

## Supervisory Board (2012)

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Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V., Munich

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Ministerium für Innovation, Wissenschaft und Forschung: Institutionelle Forschungsförderung, Düsseldorf

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Bundesministerium für Bildung und Forschung: Referat 511 - Neue Werkstoffe und Nanotechnologie, Bonn

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Bundesanstalt für Materialforschung und -prüfung, Berlin

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Ecole Nationale Supérieure de Chimie de Paris, France

Prof. Dr. Tresa M. POLLOCK
University of California, Santa Barbara, CA, USA

Dr. Benedikt RITTERBACH
Salzgitter Mannesmann Forschung GmbH, Salzgitter

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Dr.-Ing. Michael STEINHORST (membership pending)
Tata Steel Research, Development & Technology, Ijmuiden, The Netherlands

Prof. Dr. Adrian SUTTON
Imperial College London, UK

Dr. Sven VANDEPUTTE
OCAS - Arcelor Research Industry Gent, Zelzate, Belgium

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Prof. Dr.rer.nat. Jörg NEUGEBAUER (since Nov. 2004)
Prof. Dr.-Ing. Dierk RAABE (since July 1999) *
Prof. Dr.rer.nat. Martin STRATMANN (since Jan. 2000)

* chief executive since 29 Sep. 2010

**Max Planck Fellow:**
Prof. Dr.-Ing. Gunther EGGELER, Ruhr-Universität Bochum

**External Scientific Member:**
Prof. Dr. Mats HILLERT, Stockholm, Sweden
Prof. Dr. Reiner KIRCHHEIM, Göttingen

# Guest Scientists

## Computational Materials Design

Prof. Mark Asta (USA), University of California and Lawrence Berkeley National Laboratory, Berkeley, CA; July 2012

Klaus-Dieter Bauer (Austria), Johannes-Kepler-Universität Linz; Macke Scholarship Awardee; April to July 2011

Dr. Miguel Morales-Silva (USA), Lawrence Livermore National Lab; Aug to Sep. 2012

Jassel Majevadia (UK), Imperial College London; Jan. to Feb. 2012

Dr. Chris Race (UK); Alexander-von-Humboldt-Foundation; since Sep. 2011

Prof. George Smith (UK), University of Oxford; Nov. 2011

Prof. Adrian Sutton (UK), Imperial College London; Oct. 2011

Jianchuan Wang (China), Central South University, Changsha; Jan to Dec 2011

Siyuan Zhang (China), University of Cambridge, UK; German Academic Exchange Service (DAAD); Jan. 2011 to July 2012

## Interface Chemistry and Surface Engineering

Dr. Waleed Azzam (Jordan), Tafila Technical University; German Research Foundation (DFG); June to Aug. 2011

Xiaxia Bai, M.Sc. (China), Graduate University of Chinese Academy of Sciences; PhD exchange student; since Sept. 2012

Dr. Ying Chen (China); Center for Electrochemical Sciences (CES), Bochum; Feb. 2010 to Sep. 2012

Prof. Chiafu Chou (Taiwan), Institute of Physics, Academia Sinica, Taipei; German Academic Exchange Service (DAAD); Feb. 2012

Jeyabharathi Chinnaya, M.Sc. (India), CSIR-Central Electrochemical Research Institute, Tamilnadu; German Academic Exchange Service (DAAD); Oct. 2011 to Sep. 2012

Prof. Pritam Deb (India), Tezpur University, Napaam, Sonitpur, Assam; Max Planck India Fellow; July to Aug. 2011

Ashwin Anthony Fernandes, B.Sc (India), National Institute of Technology Karnataka (NITK), Surathkal; German Academic Exchange Service (DAAD) Working Internships in Science and Engineering (WISE) fellow; May to July 2011

Chethana Gadiyar, B.Sc (India), National Institute of Technology Karnataka (NITK), Surathkal; German Academic Exchange Service (DAAD) Working Internships in Science and Engineering (WISE) fellow; May to July 2012

Julien Gagnon, B.Sc. (Canada), McGill University, Montreal; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to Aug. 2012

Carolina Galeano, M.Sc., Max-Planck-Institut für Kohlenforschung, Mülheim; PhD exchange student, Jan. to Apr. 2012

Nejc Hodnik, M.Sc. (Slovenia), National Institute of Chemistry, Ljubljana; visiting PhD Student; Oct. 2010 to May 2011

Izzudin Hubby, M.Sc. (Indonesia), Research Center for Physics, Indonesian Institute of Sciences (LIPI), Jakarta; German Academic Exchange Service (DAAD); since May 2010

Dr. Maciej Krzywiecki (Poland), Assistant Professor, Institute of Physics, Silesian University of Technology, Gliwice; July to Aug. 2012

Huachu Liu, M.Sc. (China), School of Materials Science and Engineering, Shanghai University; State Scholar Fund of China; Oct. 2010 to Sept. 2011

Erin Martin, B.Sc. (USA), University of Missouri, Columbia, MU; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to July 2012

Prof. Kamachi Mudali (India), Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu; Max Planck scholarship; June 2012

Prince Nagra, B.Sc. (Canada), University of Toronto; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to Aug. 2011

Dr. Christian Schwieger, Institute of Chemistry, Martin-Luther-Universität Halle-Wittenberg; Apr. 2012

Jonathon Witte, B.Sc. (USA), Harvey Mudd College, Claremont, CA; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to Aug. 2011

## Microstructure Physics and Alloy Design

Prof. Hamid Assadi (Iran), Tarbiat Modares University, Teheran; scholarship Alexander-von-Humboldt-Foundation (AvH); July 2011 to April 2012

Li-Hui Cheng, M.Sc. (Taiwan) National Taiwan University, Taipe; German Academic Exchange Service (DAAD); May to Oct. 2011

Prof. Shoji Goto (Japan), Akita University, Akita; scholarship Alexander-von-Humboldt-Foundation (AvH); Aug. to Nov. 2011 and May to June 2012

Dr. Nan Jia (China), Northeastern University, Shenyang; scholarship Alexander-von-Humboldt-Foundation (AvH); Nov. 2010 to June 2012

Dr. José A. Jiménez (Spain), Universidad Madrid and CENIM; July to Sep. 2011, Feb. to Mar. 2012 and July to Aug. 2012

Prof. Satoru Kobayashi (Japan), National Institute of Materials Sciences (NIMS), Tsukuba; Feb. to Mar. 2012

Julio Millán, M.Sc. (Venezuela) Universidad Simón Bolívar, Caracas; German Academic Exchange Service (DAAD); April 2008 to Mar. 2012

Dr. Motomichi Koyama (Japan), National Institute of Materials Sciences (NIMS), Tsukuba; Sep. to Oct. 2011

Prof. Riccardo Lebensohn (USA), Los Alamos National Laboratory, Los Alamos; Alexander-von-Humboldt Award (AvH); Feb. 2010 to Jan. 2011

Dr. Yujiao Li (China), on leave from University of Göttingen; Jan. 2011 to Sep. 2012

Dr. Sumantra Mandal (India), Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu; scholarship Alexander-von-Humboldt-Foundation (AvH); since Apr. 2012

Dr. Ross Marceau (Australia), The University of Sydney; scholarship Alexander-von-Humboldt-Foundation (AvH); since July 2011

Prof. Nobuo Nakada (Japan), Kyushu University, Fukuoka; Japan Society for the Promotion of Science (JSPS); Oct. 2011 to Sep. 2012

Dean Pierce, M.Sc. (USA), Vanderbilt University, Nashville; funding by DFG SFB 761 ‘Stahl *ab initio*’; Mar. to May 2011 and May to July 2012

Prof. Hugo Sandim (Brazil), Escola de Engenharia de Lorena, University of São Paulo, Lorena; Aug. 2011 to Feb. 2012

Dr. Maria Sandim (Brazil), Escola de Engenharia de Lorena, University of São Paulo, Lorena; Aug. 2011 to Feb. 2012

Dr. Rodrigo Siqueira (Brazil), Escola de Engenharia de Lorena, University of São Paulo, Lorena; July to Aug. 2011 and Mar. to April 2012

Prof. Bob Svendsen (USA/Germany), on leave from RWTH Aachen; since Mar. 2012

Dr. Yun Takahashi (Japan), Nippon Steel; Apr. 2011 to Mar. 2012

Dr. Cem Tasan (Turkey), M2i, Foundation Materials Innovation Institute, Delft, The Netherlands; Mar. 2010 to Jan. 2012

Dr. Ilana Timokhina (Australia), Deakin University, Geelong, Victoria; May to Dec. 2012

Yuki Toji, M.Sc. (Japan), JFE Steel Corp. Fukuyama; since Oct. 2011

Dr. Kim Verbeken (Belgium); Ghent University; scholarship of the Research Foundation Flanders; Oct. 2007 to Sep. 2012

Prof. Yuhua Wen (China), Sichuan University, Chengdu; scholarship Alexander-von-Humboldt-Foundation (AvH); Oct. 2010 to Sep. 2011

Prof. James E. Wittig (USA), Vanderbilt University, Nashville; funding by DFG SFB 761 ‘Stahl *ab initio*’; May to July 2012

Prof. Seonghoon Yi (Korea), Kyungpook National University, Daegu; Mar. 2011 to Feb. 2012

Dr. Han Zhang (China), Tsinghua University, Beijing; scholarship Alexander-von-Humboldt-Foundation (AvH); since Dec. 2011

Dr. Chengwu Zheng (China), Institute of Metal Research, Chinese Academy of Sciences, Shenyang; scholarship Alexander-von-Humboldt-Foundation (AvH); Mar. 2010 to Feb. 2012

# Scientific Honours

## *2010 (not included in Scientific Report 2009/2010)*

*Dr. C. Herrera* obtained the Best Poster Award at the 4th International Conference on Recrystallization and Grain Growth, Sheffield, UK, 4-9 July 2010.

*Dr. A. Kostka* was honourably mentioned in the micrograph competition “The Art behind the Science” at the International Microscopy Congress IMC 17, Rio de Janeiro, Brazil, Sep. 2010.

*Prof. Dr. J. Neugebauer* became an elected member of the North Rhine-Westphalian Academy of Sciences, Mar. 2010.

*Prof. Dr. D. Raabe* was called by the German Bundespräsident as a member of the German Science Advisory Board (Wissenschaftsrat), Febr. 2010.

*N.H. Siboni* passed his master thesis about “Statistical and quantum mechanical simulation of interstitials in metals: mechanisms and constraints for superabundant vacancy formation” with excellence. RWTH Aachen, Dec. 2010.

## *2011*

*V. Becker* has achieved the 1st place in the Programming Competition 2010/2011 of the Mathe-dual e.V., Mar. 2011.

*U. Benedikt* won the 2nd Best Poster Prize on the 47th Symposium for Theoretical Chemistry, Sursee, Switzerland, Sep. 2011.

*Dr. P. Choi* has received the Golden Poster Award for the poster “Nanoscale characterization of TiAlN/CrN multilayer hard coatings” at the 5th International Union of Microbeam Analysis Societies meeting, Seoul, Korea, 22-27 May, 2011.

*N.-N. Elhami* and *Dr. S. Zaefferer* have won the 1st Poster Prize of the Royal Microscopical Society at the RMS-EBSD 2011 conference for the poster "Interpretation and application of cECCI Images for defect analysis in TWIP steels", London, UK, Mar. 2011.

The article by *Dr. B. Grabowski, Dr. T. Hickel, Prof. Dr. J. Neugebauer* “Formation energies of point defects at finite temperatures”, Phys. Status Solidi B 248 (2011) 1295, was selected for the front cover.

The article by *Dr. T. Hickel, Dr. B. Grabowski, Dr. F. Körmann* and *Prof. Dr. J. Neugebauer*, “Advancing DFT to finite temperatures: Methods and applications in steel design”; Psi-k Newsletter 105 was selected as highlight for the Psi-k newsletter, June 2011.

*Dr. S.O. Klemm* received the Dr. Klaus Seppeler Stiftungspreis 2011 of the GfKORR Deutsche Gesellschaft für Korrosionsschutz e.V., Nov. 2011.

*Dr. F. Körmann* passed his doctoral thesis “Magnetic systems studied by first-principles thermodynamics” with excellence, University of Paderborn, May 2011.

*Dr. R. Marceau* from Sydney (Australia) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Aug. 2011.

*Dr. K.J.J. Mayrhofer* was awarded a grant about 1 million Euro from the Federal Ministry of Education and Research for his project “ECCO$_2$”, Nov. 2011.

*Dr. K.J.J. Mayrhofer* received the Anton-Paar Prize (Junior scientist prize < 35) of the Austrian Chemical Society GÖCH, Linz, Austria, Sep. 2011.

*Prof. Dr. D. Raabe* was awarded the DGM Prize from the Deutsche Gesellschaft für Materialkunde as excellent researcher for outstanding scientific or scientific-technical achievements in materials science and materials engineering, 15 June 2011.

*Dr. C. Race* from London (UK) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Sep. 2011.

*Dr. F. Roters* has successfully completed his habilitation at the RWTH Aachen, faculty 5: Georessourcen und Materialtechnik with the lecture: "Werkstoffe für den Computer von Morgen". His habilitation dissertation is entitled: "Advanced Material Models for the Crystal Plasticity Finite Element Method - Development of a general CPFEM framework". The right to teach (*venia legendi*) was granted for “Computational Material Science”, Aachen, June 2011.

*Dr. S. Sandlöbes* has been awarded the Borchers-Plakette of the RWTH Aachen for her excellent doctoral thesis about "Untersuchungen zum Einsatz berührungsloser in-situ Messmethoden metallurgischer Gase". Aachen, 16 June 2011.

## 2012

*Dr. O. Cojocaru-Mirédin* is one of the winners of the competition “NanoMatFutur” with a grant of 1.3 million Euro, May 2012.

*Prof. Dr. G. Dehm* got an appointment for an extraordinary professorship (außerplanmäßige Professur) at the Ruhr-Universität Bochum, Nov. 2012.

*Dr. M. Herbig* has been selected for the best poster prize of the “Solid-State Interfaces II: Towards an Atomistic-Scale Understanding of Structure, Properties, and Behaviour through Theory and Experiment” Symposium at the TMS 2012 Annual Meeting & Exhibition in Orlando, FL, USA, Mar. 2012.

*D. Korbmacher* passed his master thesis “Dual scale modelling of hydrogen embrittlement” with excellence. Ruhr-University Bochum, Aug. 2012.

*C. Jacobs* was awarded the Azubipreis of the Max Planck Society for being the best apprentice in the district Duisburg/Solingen in the field of material testing. Munich, Sep. 2012.

*Dr. F. Körmann* obtained the Otto-Hahn-Medal of the Max-Planck Society, Düsseldorf, June 2012.

*Dr. F. Körmann* obtained the CALPHAD Poster Award, Berkeley, CA, USA, June 2012.

*Dr. B. Lange* passed his doctoral thesis “p-Dotierbarkeit von Galliumnitrid” with excellence. University of Paderborn, Aug. 2012.

*Dr. S. Mandal* from Kalpakkam (India) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Apr. 2012.

*Dr. K.J.J. Mayrhofer* received the ISE Prize for Applied Electrochemistry (Junior scientist prize < 35) of the International Society of Electrochemistry ISE. Santiago de Queretaio, Sep. 2012.

*Dr. K.J.J. Mayrhofer* received the ‘Innovationspreis des Landes NRW in der Kategorie „Nachwuchs“‘ (innovation award of the state NRW in the category “junior scientists”), Nov. 2012.

*J. Meier* obtained the Best Poster Prize of the 63rd Annual Meeting of the ISE in Prague, Czech Republic, Aug. 2012.

*Prof. Dr. J. Neugebauer* and *Prof. Dr. D. Raabe* have jointly received an ERC Advanced Grant for their research project SMARTMET from the European Research Council. The award is worth 3 million Euro, 24 Jan. 2012.

*Prof. Dr. J. Neugebauer* has been elected as member of the “DFG-Fachkollegium 302 Chemische Festkörper- und Oberflächenforschung, Theorie und Modellierung”, Feb. 2012.

*Prof. Dr. J. Neugebauer* became a member of the IT strategy group of the Max Planck Society, Apr. 2012.

*Prof. Dr. D. Raabe* was elected as member and chairman of the Hochschulrat (Board of Governors) of RWTH Aachen University, Aachen, Nov. 2012.

*A. Schuppert* has received the ‘Nachwuchspreis’ of the association ZELLCHEMING (Zellstoff- und Papierchemiker und -Ingenieure e.V.), Wiesbaden, June 2012.

*Dr. S.Y. Shin* from Pohang (Korea) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Apr. 2012.

*N. Tillack* passed her master thesis “Chemical trends in the yttrium-oxide precipitates in oxide dispersion strengthened steels: A first-principles investigation” with excellence. Ruhr University Bochum, Mar. 2012.

*PD Dr. S. Zaefferer* received an offer for a position as professor on the chair for electron microscopy and scientific director of the Center for Electron Nanoscopy, Technical University Kopenhagen, Denmark, Apr. 2012.

*PD Dr. S. Zaefferer* received an offer for a position as professor on the chair for physical metallurgy, Technical University Wien, Austria, May 2012.

*Dr. H. Zhang* from Beijing (China) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Jan. 2012.

The *MPIE* was honoured by the Düsseldorf Chamber of Commerce and Industry (IHK Düsseldorf) for its excellent performance in occupational training (Nov. 2012).

# Participation in Research Programmes

## National:

**BMBF (Federal Ministry of Education and Research)**

Combinatorial electrocatalytic $CO_2$ reduction

Development of ferritic steels for high-temperature applications

Increase of competence in electrochemistry for electromobility

Novel corrosion protection coatings compatible with hot forming

Ultra-high resolution EPR spectroscopy on thin film silicon for solar cell research (EPR-Solar)

**BMWi (Federal Ministry of Economics and Technology)**

Hydrogen induced embrittlement of hardened cold rolls (IWAS)

Next Generation MKWS - Development of corrosion-resistant and expansion-adapted micro channel heat sinks for high-power diode lasers - Selection and qualification of materials

**DAAD (German Academic Exchange Service)**

Investigation of the behaviour of water in confined geometries

**DFG (German Research Foundation)**

*Ab initio* and atomistic calculations of complex bio-materials

*Ab initio* based description of hydrogen embrittlement

*Ab initio* description of temperature dependent effects in dimensionally constrained magnetic shape memory Heusler alloys (SPP)

*Ab initio* determination of free energies and derived properties (Heat capacities, vacancies, solvus boundaries) for selected Al alloys containing Si, Mg and Cu

*Ab initio* investigation of temperature-driven martensitic transformations: Case study for alkali earth metals

*Ab initio* study on the coupling of lattice and magnetic degrees of freedom and the role of interfaces in magneto-caloric materials

Algorithms for the fast materials-oriented simulation of process chains in forming technology (SPP 1204)

Antireflecting interlayers to increase transmission through thin metal films in spectroelectrochemical experiments

Atomic scale investigation of compositional changes at interfaces using Atom Probe Tomography

Atomic scale investigation of the kinetics of nano-precipitation in Fe–Si–Cu alloys using Atom Probe Tomography

Biomimetic photonic crystals with mechanochromic properties based on cuticular scales of the weevil *Entimus imperialis.*

Characterization and modeling of the interplay between grain boundaries and heterogeneous plasticity in titanium

Characterization of $Cu(In,Ga)Se_2$ thin-film solar cells by means of atom probe tomography

Constitutive modeling and microstructural validation for crystal plasticity finite element computation of cyclic plasticity in fatigue

Crustacean skeletal elements: variations in the constructional morphology at different hierarchical levels

Deformation mechanisms and local residual stresses in the system Fe–Mn–C (SFB)

Development and validation of a multiscale description of heterogeneous deformation and inter-crystalline fracture of molybdenum

Elastic effects on heterogeneous nucleation and microstructure formation

Elucidation of corrosion phenomena with high lateral resolution using scanning probe techniques

Experimental and theoretical investigations of the dynamics of collective phenomena in blood I: Idealized vesicle/fluid droplet models

Fine lamellar Fe–Al *in situ* composite materials: Microstructure and mechanical properties

Fundamental investigation of the mechanisms of deformation and recrystallisation of cold deformable Mg alloys micro-alloyed with rare earth elements and microstructure optimization for the development of a new class of Mg-alloys.

Heapocrates: Healing polymers for preventing corrosion of metallic systems

High resolution scanning electron back scatter diffraction experiments of local crystallographic orientation patterning during plastic deformation

Highly accurate calculation of parameters of the NMR spectroscopy, development, benchmarking and application

Investigation and characterization of the intermetallic phase formation of dissimilar FeAl-joints produced by fast laser-based joining processes with large temperature gradients

Investigation of local alloy compositions by atom probe tomography

Limits and controllability of the impurity level of titanium recycling alloys for further use

Local mechanical properties of Mn-based steels (SFB)

Manufacturing, structural characterization and investigation of the mechanical properties of ultra fine grained and nanocrystalline structured $Fe_3Al$–X (X=Cr, Ti) alloys

Materials World Network: Physically based approach for predicting and minimizing damage nucleation in metals

Mechanisms of self and impurity diffusion in Fe–Al intermetallic compounds

Microbially induced corrosion by sulfate-reducing bacteria

Microstructure mechanics and fundamentals of concurrent twinning and martensite formation (SFB)

Nanofluid mechanics

Quantum mechanically guided design of ultra strong glasses

Scale-bridging studies of the elastic contributions to nucleation and initial microstructure formation in the eutectic system Ti–Fe

Steel - *ab initio*: Quantum-mechanically guided design of new Fe-based alloys partial project: “Defects and residual stresses in Fe–Mn–C steels” (SFB 761/1 partial project C05)

Steel - *ab initio*: Quantum-mechanically guided design of new Fe-based alloys partial project: “*Ab initio* derivation of Gibbs enthalpies, stacking fault energies and boundary energies at finite temperatures” (SFB 761/1 partial project A02)

STM characterization of novel SAMs

Synthesis and characterization of reference materials (SFB)

Thermal stability of metal nitride superlattices studied by means of atom probe tomography

**Helmholtz Society**

Improving performance and productivity of integral structures through fundamental understanding of metallurgical reactions in metallic joints (IPSUS)

Ultra-high resolution EPR spectroscopy on thin film silicon for solar cell research (EPR-Solar)

**Max Planck Society**

Active coatings for corrosion protection (ASKORR)

Characterisation of iron oxide nanoparticles

Computational mechanics of polycrystals

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

Triple-M: Max Planck initiative on multiscale materials modeling of condensed matter

**State of North Rhine-Westphalia**

Center for Electrochemical Sciences (CES)

High-pressure Fe–Al steam turbine blade - Development of a processing route for fabrication of a high-pressure iron aluminide steam turbine blade

Innovative materials development for cutting tools by the strip casting manufacturing technique - Bladestrip

## International:

**Christian Doppler Society**

Diffusion and segregation mechanisms during production of high strength steel sheet, Module I: Selective enrichmenet at hot and cold rolled strip

Diffusion and segregation mechanisms during production of high strength steel sheet, Module II: Pickling Module

Diffusion and segregation mechanisms during production of high strength steel sheet, Module III: Hydrogen Module

**European Union**

Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys (SMARTMET)

AlGaInN materials on semi-polar templates for yellow emission in solid state lighting applications

Novel concepts for molecular interface engineering and unravelling of structure/property relationships at electrified interfaces (MultiScAd)

Surface engineered InGaN heterostructures on N-polar GaN-substrates for green light emitters

**Foundation Materials Innovation Institute**

Development of full field gradient plasticity FEM code to predict constitutive material model for dual phase steels

Mobility of water and charge carriers in polymer/oxide/aluminium alloy interfaces

Mechanics of phase boundaries in multi-phase steels

**RFCS**

Advanced zinc-based hot dip coatings for the automotive application (AUTOCOAT)

High emissivity annealing technique (HEAT)

Hydrogen sensitivity of different advanced high strength microstructures (HYDRAMICROS)

New approaches to quantitative hydrogen analysis of coated steel products (COATHYDRO)

New developments and optimisation of high strength boron treated steels through the application of advanced boron monitoring techniques (OPTIBOS)

Steady reactivity in hot-dip coating by direct deposit of iron oxides

**Sino-German Center for Research Promotion**

Liquidus surfaces and reaction schemes of the ternary systems Cr–Al–Nb and Fe–Al–Nb: Experiments and thermodynamic modelling

Mechanisms of self and impurity diffusion in Fe–Al intermetallic compounds

# Conferences, Symposia and Meetings Organized by the Institute

## *2011*

*T. Hickel and R. Spatschek* co-organized the sessions “Thermodynamic modeling” and “Kinetics of phase transitions”, respectively, of the “Advanced Discussions, Current Developments” meeting, which took place at Ruhr-Universität Bochum, 10 and 11 Mar. 2011.

*P. Choi* organized the Bilateral Korean-German workshop between Korea Institute of Science and Technology (KIST) and MPIE, which was held at MPIE on 25 Mar. 2011. 10 lectures were given to about 50 participants.

*T. Hickel and J. Neugebauer* organized a focus meeting of the SPP1239 on "Fundamentals of shape-memory alloys" at MPIE Düsseldorf, 13 and 14 Apr. 2011.

*A. Bobrowski and H. Bögershausen* organized the conference “Mikroskopie und Präparation 2011 - MikPräp 2011” of the Gesellschaft für Materialografie Rhein - Ruhr (GMR$^2$), Solingen, 14 Apr. 2011.

*L. Lymperakis and R. Spatschek* organized the Computational Materials Design Workshop in Attendorn, 6 to 8 July 2011.

*S. Sandlöbes* organized the meeting of the “Arbeitskreis Konstruktionswerkstoffe" of the “DGM Fachausschuss Mg” which took place at MPIE on 6 Oct. 2011.

*M. Rohwerder* organized and chaired the 220th ECS Meeting “Coatings for Corrosion Protection” in Boston, MA, USA, 9 to 14 Oct. 2011.

*L. Lymperakis* co-organized the SINOPLE Nitrid Workshop at the Harnack-Haus, Berlin, 12 and 13 Oct. 2011.

*C. Freysoldt* co-organized the EPR Solar Workshop at the Helmholtz-Zentrum Berlin, 13 and 14 Oct. 2011.

*C. Freysoldt* organized a workshop on “Modern developments in the *ab initio* description of charged systems for semiconductors and electrochemistry” at Ringberg castle, 23 to 26 Oct. 2011.

*C. Tasan* organized the “MPIE Workshop on Dual-Phase Steel”, which was held at MPIE on 24 Nov. 2011. 10 lectures were presented to about 80 participants from industry and universities.

## *2012*

*J. von Pezold* organized the 1st Austrian-German workshop on Computational Materials Design in Kramsach, Austria, 23 to 27 Jan. 2012.

*M. Palm* organized and chaired the 20th meeting of the “Fachausschuss Intermetallische Phasen (FA-IP)” which was held at MPIE on 23 Feb. 2012. 6 talks were given to about 40 participants.

*A. Erbe* organized together with SENTECH Instruments the seminar "Thin Film Metrology" at the MPIE, 1 Mar. 2012.

*J. Neugebauer* organized a symposium at the DPG Spring Meeting on “Materials design on the atomistic scale: Experiment meets theory”, Berlin, 25 to 30 Mar. 2012.

*T. Hickel and R. Spatschek* co-organized the sessions “Thermodynamic modeling” and “Kinetics of phase transitions”, respectively, of the “Advanced Discussions, Current Developments” meeting, Ruhr-Universität Bochum, 26 and 27 Apr. 2012.

*T. Hickel, C. Race, R. Drautz and J. Neugebauer* organized a workshop on "*Ab initio* Description of Iron and Steel: Thermodynamics and Kinetics (ADIS)” at Ringberg castle, 29 Apr. to 5 May 2012.

*M. Herbig* organized the “MPIE Workshop on Hydrogen Embrittlement in Steels” at MPIE on 25 June 2012. 8 lectures were presented to about 120 participants from industry and universities.

*P. Eisenlohr* organized the “3rd International Symposium Computational Mechanics of Polycrystals” which was held in Bad Honnef on 28 and 29 June 2012. More than 20 talks were given to about 45 participants from 7 countries.

*J. Neugebauer* co-organized the Joint European Condensed Matter Conferences CMD-24 - CMMP-12 - ECOSS-29 - ECSCD-11, Edinburgh, UK, 3 to 9 Sep. 2012.

*J. Neugebauer* was a member of the Technical Committee at the Hydrogen Conference “Hydrogen-Materials Interactions”, Wyoming, WY, USA, 9 to 12 Sep. 2012.

*J. Neugebauer* co-organized the ECCOMAS Symposium “Computational design of functional thin films”, Wien, 10 to 14 Sep. 2012.

*J. Neugebauer* organized a symposium “Multiscale Modelling of Mechanical Properties” at the MSE Darmstadt, 25 to 27 Sep. 2012.

*J. Neugebauer* co-organized a joint symposium “Thermodynamic Concepts in Materials & Process Design” at the MMM Singapore, 15 to 19 Oct. 2012.

# Institute Colloquia and Invited Seminar Lectures

## *2011*

*P. Rehak*, Brno University of Technology, Brno, Czech Republic: Study of Dynamical Stability of Crystals (5 Jan. 2011)

*W. Shan*, University of Hannover: Coupled Finite Element-Lattice Static Model, with Adaptivity (10 Jan. 2011)

*S. Brinckmann*, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum: Towards Combining Molecular Dynamics and Discrete Dislocation Dynamics (31 Jan. 2011)

*H.J. Maier*, Universität Paderborn: Microstructure and Mechanical Properties of Conventional and Magnetic Shape Memory Alloys (2 Feb. 2011, Colloquium)

*N. Marzari*, University of Oxford, UK: Simple Solutions to Complex Problems: Towards High-Throughput Screening of Novel Thermoelectrics and Ferroelectrics (14 Feb. 2011)

*J. Repper*, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TU München: Intergranular Residual Stress Studies and More by Neutron Diffraction (15 Feb. 2011)

*P.V. Satyam*, University of Bremen: Compositional Analysis of SiGe Nanostructures by Electron and Ion Scattering Methods (16 Feb. 2011)

*V. Komanicky*, Safarik University, Kosice, Slovakia: Electrocatalysis on Precisely Tailored Nano-Sized Model Systems (23 Feb. 2011)

*J. Senger*, Karlsruhe Institute of Technology (KIT): Discrete Dislocation Dynamics Simulations of Mechanical Properties in Micrometer Sized Pillars (24 Feb. 2011)

*M.J. Duarte Correa*, Cinvestav IPN, Querétaro, Mexico and Universitat Politècnica de Catalunya, Castelldefels, Spain: Preparation and Characterization of Structure and Stability of Different Metallic Glasses (3 Mar. 2011)

*L. Ismer*, University of California, Santa Barbara, CA, USA: Point-Defect-Mediated Dehydrogenation of $AlH_3$, (8 Mar. 2011)

*A. Terfort*, Goethe-Universität Frankfurt/Main: Self-Assembled Monolayers as Functional Materials (15 Mar. 2011, Colloquium)

*M. Griebel*, Universität Bonn: Numerical Simulation in Material Science and Nanotechnology (24 Mar. 2011)

*G. Schütz*, Max-Planck-Institut für Intelligente Systeme, Stuttgart: X-Ray Microscopy in Material, Environmental Science and Biology (31 Mar. 2011)

*G. Dehm*, Montanuniversität Leoben, Austria: New Insights in Plasticity of Metals by Highly Localized *in situ* Measurements (1 Apr. 2011, Colloquium)

*T. Schena*, Forschungszentrum Jülich: Tight-Binding Treatment of Complex Magnetic Structures in Low-Dimensional Systems (1 Apr. 2011)

*C. Scheu*, Ludwig-Maximilians Universität München: Atomic Scale Analysis of Nanostructures and Interfaces (19 Apr. 2011, Colloquium)

*S. Baldelli*, University of Houston, TX, USA: Sum Frequency Generation Vibrational Spectroscopic Imaging of Monolayers on Surfaces (28 Apr. 2011)

*I. A. Abrikosov*, Linköping University, Sweden: Towards Predictive Theory for *ab initio* Simulations of Materials Properties (4 May 2011)

*S. Chakraborty*, Ruhr-Universität Bochum: Silicon Revisited with an *ab-initio* Approach (1 June 2011)

*S. Wege*, Leibnitzinstitut für Werkstoffwissenschaft (IfW), Dresden: Method for Determination of Strain in Polycrystals using EBSD (9 June 2011)

*E. Quandt*, Institute for Materials Science, Christian-Albrechts-Universität zu Kiel: Thin Film Smart Materials for Medical Applications (4 July 2011, Colloquium)

*I. Bleskov*, CIRIMAT-ENSIACET-INP, Toulouse, France: Theoretical Investigation of Elastic Properties of New Refractory RuAl-Based Alloys (5 July 2011)

*F. Otto*, Max Planck Institute for Mathematics in the Sciences, Leipzig: Pattern Formation in Micromagnetics (11 July 2011)

*E. Spohr*, University Duisburg-Essen: Simulating Proton Transfer to Metal Electrodes with Reactive Molecular Dynamics Trajectories (12 July 2011, Colloquium)

*Y. Cui,* Paris, France: p-type Doping and Codoping of ZnO Based on Nitrogen is Ineffective: An *ab initio* Clue (12 July 2011)

*E. Kabliman*, Vienna University of Technology, Austria: *Ab initio*-Based Mean Field Theory of the Site Occupation in the Fe-Cr Sigma Phase (18 July 2011)

*A. Winkelmann*, Max Planck Institute for Microstructure Physics, Halle: The Physics of EBSD (27 July 2011)

*D. Haley*, University of Oxford, UK: Curvature Flow for Dynamic Emitter Geometry in Atom Probe (29 Aug. 2011)

*R.C. Reed*, University of Birmingham, UK: Nickel-Based Superalloys: Construction, Use and Validation of Numerical Models (1 Sep. 2011, Colloquium)

*H. Assadi*, Tarbiat Modares Univerisity, Tehran, Iran: Cold Spray Technology - Thermal Spraying on the Verge of Metal Forming (5 Sep. 2011)

*D. Lambrecht*, University of California, Berkeley, CA, USA: Multi-Scale Electronic Structure Simulation of Soft Matter and Chemistry at Interfaces (16 Sep. 2011)

*D. Usvyat*, University of Regensburg: Towards an Accurate Theoretical Description of Physisorption: Periodic Local-Correlation Method (27 Sep. 2011)

*L. Nykänen*, University of Jyväskylä, Finland: Chemistry of Carbon on Transition Metal Surfaces (27 Sep. 2011)

*Y. Bar Sinai*, Weizmann-Institut, Rehovot, Israel: Slow Rupture in a Generic Friction Model (29 Sep. 2011)

*J.B. Seol*, POSTECH Pohang University of Science and Technology, South Korea: 1. Role of Carbon Atoms on the Deformation Behavior of Strain-Induced Martensites in the High Mn Steels; 2. Atomic Scale Investigation on (Fe,Mn)$_3$AlC Carbides Formed in High Aluminum Transformation-Induced-Plasticity Steels by Atom Probe Tomography (29 Sep. 2011)

*P. Sofronis*, International Institute for Carbon-Neutral Energy Research, Kyushu University, Fukuoka, Japan, and University of Illinois at Urbana-Champaign, IL, USA: International Institute for Carbon-Neutral Energy Research - Outline and Future Perspectives (6 Oct. 2011)

*K. Tsuzaki*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Structural Materials Research at NIMS (10 Oct. 2011)

*S. Kobayashi*, National Institute for Materials Science (NIMS), Tsukuba, Japan: The Effect of Grain Boundary Precipitates on High Temperature Strength in Fe$_3$Al Based Alloys (11 Oct. 2011)

*D. Rettenwander*, Universität Salzburg, Austria: Computational Characterization of Methionine Radicals (17 Oct. 2011)

*A. Sutton*, Imperial College London, UK: The Theory of Grain Boundary Structure in Single-Component and Multi-Component Crystals (18 Oct. 2011, Colloquium)

*S. Naghavi*, Johannes Gutenberg Universität Mainz: Elastic Properties of Heulser Compounds from First-Principle Calculations (19 Oct. 2011)

*W.A. Curtin*, Brown University, Providence, RI, USA: From Atoms to Ductility: the Mechanisms of Dynamic Strain Aging and its Impact on Ductility in Al-Mg Alloys (7 Nov. 2011)

*W.A. Curtin*, Brown University, Providence, RI, USA: First-principles Predictions of Solute Strengthening in Al and Mg Alloys (8 Nov. 2011)

*M. Mehring*, Technische Universität Chemnitz: Molecular Precursors and Clusters for the Synthesis of Metal Oxides and Organic-Inorganic Hybrid Materials Containing Bismuth (8 Nov. 2011, Colloquium)

*G. Smith*, University of Oxford, UK: Where are the Carbon Atoms in Martensite? (15 Nov. 2011, Colloquium)

*A. Klamt*, COSMOlogic GmbH&CoKG, Leverkusen, and University of Regensburg: COSMO-RS, the Bridge from Quantum Chemistry to Fluid Phase Thermodynamics (16 Nov. 2011)

*G. Smith*, University of Oxford, UK: Where are the Carbon Atoms in Martensite? Continued (17 Nov. 2011)

*D. Zaytsev*, Ural Federal University Ekaterinburg, Russia: The Relationship between Mechanical Properties and Microstructure of Human Tooth Hard Tissues (22 Nov. 2011)

*J. Takahashi*, Advanced Technology Research Labs, Nippon Steel Corporation, Chiba, Japan: Application of Atom Probe Tomography Analysis to Traditional Issues of Steel Materials (23 Nov. 2011)

*W. Poole*, University of British Columbia, Vancouver, Canada: Developing Magnesium Materials for the Transportation Sector - An Overview of the Canadian Research Network, MagNET (28 Nov. 2011)

*D. Holec*, Montanuniversitaet Leoben, Austria: Electron Energy Loss near Edge Structures of AlN-Based Ternary Thin Films: Theory vs. Experiment (29 Nov. 2011)

*P. Neumann*, Mettmann, retired (former director at MPIE): Calculating the Giant Strains at the Intersections of Slip Bands (29 Nov. 2011, Colloquium)

*G. Zimbitas*, TU Delft, The Netherlands: Internal Oxidation of Binary Ni Alloys (29 Nov. 2011)

*A. Chakrabarty*, Trinity College Dublin, Irland: Role of Defects and Impurities in Ferromagnetic Oxides: An Electronic Structure Study (30 Nov. 2011)

*K. Murgaeva*, TU Bergakademie Freiberg: TEM Analysis of the Orientation Relationships and Interfaces in Nanocomposites (1 Dec. 2011)

*R. Schuster*, Karlsruhe Institute of Technology (KIT), Karlsruhe: Electrochemical Microcalorimetry (6 Dec. 2011, Colloquium)

*M. Rizzi*, Ecole Polytechnique Federale de Lausanne, Switzerland: Carbon Dioxide Adsorption and Hydrogenation on Nickel-Based Surfaces: A First Principles Study (7 Dec. 2011)

*P. Dey*, Indian Institute of Technology Guwahati, India: Effect of Random Disorder on Superconductivity (13 Dec. 2011)

*M. Militzer*, University of British Columbia, Vancouver, Canada: Multi-scale Modelling of Phase Transformations in Steels (14 Dec. 2011)

*P. Neumann*, Mettmann, retired (former director at MPIE): A Heavenly Beautiful Journey into Deep Space (15 Dec. 2011)

*R. Sigel*, University Fribourg, Switzerland: Adsorption and Diffusion Dynamics at Interfaces (16 Dec. 2011)

## *2012*

*S. Chentouf*, University Paul Verlaine of Metz, France: *Ab initio* Study of the Effect of Ti and Zr Transition Metals Located in Bulk $D0_3$-$Fe_3Al$ and $\Sigma 5$ (310)[001] Grain Boundary (9 Jan. 2012)

*C. Teichert*, Montanuniversitaet Leoben, Austria: Atomic-Force Microscopy Based Electrical and Mechanical Characterization on the Nanometer Scale (10 Jan. 2012)

*H. Riechert*, Paul-Drude-Institut, Berlin: InGaN/GaN Nanowires on Si - A Viable Route towards LEDs on Si? (19 Jan. 2012)

*Z. Strelcova*, Central European Institute of Technology, Masaryk University, Brno, Czech Republic: From Bioinformatics to *ab-initio* Dynamics, From Supramolecules to Biomolecules (19 Jan. 2012)

*S. Ringer*, Australian Centre for Microscopy & Microanalysis, University of Sydney, Australia: Alloy Design guided by Advanced Atom Probe Tomography and Microstructure Characterisation (24 Jan. 2012)

*C.-H. Fischer*, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin: Spray-ILGAR (Ion Layer Gas Reaction) and Spray-Pyrolysis - Two Powerful Methods for the Deposition of High Quality Compact or Nano-Dot Thin Films (2 Feb. 2012)

*E. Arzt*, INM - Leibniz Institute for New Materials and Saarland University Saarbrücken, Germany: Bioinspired Mesotextured Surfaces for Active Surface Control (6 Feb. 2012, Colloquium)

*P.K. Nayak*, Weizmann Institute of Science, Rehovot, Israel: Effect of Material Disorder and Interfacial Energetics on Photovoltaic Efficiency (9 Feb. 2012)

*J. Weissmüller*, Technische Universität Hamburg-Harburg and Helmholtz-Zentrum Geesthacht: Novel Functional Materials Based on Nanoporous Metals (9 Feb. 2012)

*K.-U. Neumann*, Loughborough University, UK: A Structural and Electrical Resistivity Investigation of some $Cr_2VX$ and $Ni_{2-x}Mn_{1+x}Ga$ Heusler alloys (28 Feb. 2012)

*E. Spiecker*, Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg: Bridging Length Scales in Transmission Electron Microscopy of Materials (28 Feb. 2012)

*A. Schlieter*, Institute for Complex Materials IFW Dresden: Scale-Bridging Studies of the Elastic Contributions to Nucleation and Initial Microstructural Formation in the Eutectic Ti-Fe System (29 Feb. 2012)

*K. Tsuchiya*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Improvement of Strength and Ductility by Heterogeneous Microstructures (5 Mar. 2012)

*K. Verbeken*, Ghent University, Belgium: Evaluation of Hydrogen Trapping in Iron-Based Alloys by Thermal Desorption Spectroscopy (5 Mar. 2012)

*I. Watanabe*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Numerical Prediction of Deformed Microstructure Subjected to Plastic Forming with Two-Scale Finite Element Analysis (5 Mar. 2012)

*T. Ohmura*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Indentation-Induced Plasticity of Metals with Various Lattice Defects (6 Mar. 2012)

*R.C. Chiechi*, University of Groningen, The Netherlands: Unconventional Tools for Constructing Tunneling Junctions from Self-Assembled Monolayers (13 Mar. 2012, Colloquium)

*G. Bester*, Max-Planck-Institut fürFestkörperforschung, Stuttgart: Frontiers in the Atomistic Modeling of Nanostructures (15 Mar. 2012)

*G.P. Leyson*, Brown University, Providence, RI, USA: Solute Strengthening from First Principles and Application to Al and Mg Alloys (20 Mar. 2012)

*O. Cheiliakh*, Pryazovskyi State Technical University, Mariupol, Ukraine: The Creation and Strengthening of New Effective Functional Metastable Alloys Based on Effect of Phase Transformations Induced by Deformation (3 Apr. 2012)

*H. Kitaguchi*, Oxford University, UK: Carbon and Carbides in Metals: Understanding the Effect of Carbon and Carbides on Mechanical Properties and Developing a Strategy to Achieve Full Carbon Quantification using EELS and APT (4 Apr. 2012)

*S. Peljhan*, Jozef Stefan Institute, Ljubljana, Slovenia: Simulations of BTAH and Cl Adsorption on Cu Surfaces: Towards Understanding the Corrosion Inhibition Action on the Atomic Level (11 Apr. 2012)

*R. Groeger*, Academy of Sciences of the Czech Republic, Institute of Physics of Materials, Brno, Czech Republic: Atomic-Level Foundations of the Plastic Deformation of bcc Metals (24 Apr. 2012)

*S. Bargmann*, University of Dortmund: Modeling and Simulation of Polycrystalline Metals Based on Extended Crystal Plasticity (2 May 2012)

*J. Brillo*, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln: Thermophysical Properties of Liquid Multicomponent Alloys (3 May 2012)

*C. Peter*, Max Planck Institute for Polymer Research, Mainz: Hierarchical Simulations of Polyelectrolyte Solutions in Contact with Calcite Surfaces (3 May 2012)

*M. Korth*, Universität Ulm: Computational High-Throughput Screening of Advanced Battery Electrolyte Solvents (7 May 2012)

*A. Haschibon*, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg: Modeling and Simulation of Solid-Solid and Solid-Liquid Interfaces (10 May 2012)

*K. Brandhorst*, Institute for Advanced Simulation (IAS), Forschungszentrum Jülich: Mechanical Bond Strength Descriptors and Sparse Matrix Algebra (25 May 2012)

*A. Dianat*, TU Dresden: First-Principle Simulations of Materials Properties (4 June 2012)

*U. Kamachi Mudali*, Indira Gandhi Centre for Atomic Research, Kalpakkam, India: Superhydrophobic Way for Corrosion Protection of Metals and Alloys (21 June 2012)

*C.G. Levi*, University of California, Santa Barbara, CA, USA: Extending the Temperature Capability of Thermal Barrier Coatings: Fundamental Challenges and Possible Materials Solutions (26 June 2012)

*A. Breidi*, Chimie Métallurgique des Terres Rares, CNRS, Université Paris-Est, France: *Ab initio* Study of Topologically Close-Packed Phases (TCP) in Rhenium-Based Binaries (27 June 2012)

*V. Subramanya Sarma*, Indian Institute of Technology, Madras, India: Strategies for Improving the Ductility of Ultrafine Grained/Nanostructured Metals and Alloys (28 June 2012)

*G. Winther*, Technical University of Denmark, Lyngby, Denmark: Microstructure, Slip Systems and Plastic Anisotropy (2 July 2012)

*A.A. Kornyshev*, Imperial College London, UK: Ionic Liquids at Interfaces and in Confinement: From Fundamentals to the Physics of Supercapacitors and Electroactuators at the Nanoscale (3 July 2012, Colloquium)

*I. Lauermann*, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH: Synchrotron-Based Characterization of Surfaces and Interfaces in Chalcopyrite Thin Film Solar Cells (13 July 2012)

*T. Furuta*, Toyota Central R&D Labs., Inc., Aichi, Japan: Ideal Strength Metallic Materials (16 July 2012)

*T. Maeshima*, Toyota Central R&D Labs., Inc., Aichi, Japan: Microstructure of Al-TM (Transition Metal) System by Aggressive Use of Fe (16 July 2012)

*A. Barnoush*, Saarland University, Saarbrücken: Micro- and Nanomechanical Testing under Simulated Environmental Conditions (17 July 2012)

*M. Zeleny*, Aalto University School of Science, Finland: *Ab initio* Study of Magnetism of Manganese in Nanostructures and Thin Films (17 July 2012)

*S. Korte*, Friedrich-Alexander-Univerität Erlangen-Nürnberg: Plasticity in Hard Materials - Probing Deformation Mechanisms by Micromechanical Testing across Sizes and Temperatures (18 July 2012)

*Z. Wang*, Shenyang National Laboratory for Materials Science, Chinese Academy of Sciences, Shenyang, China: Aluminization Behavior and Austenitization Process of a Ferritic Heat-Resistant Steel with a Nanostructured Surface Layer (18 July 2012)

*M. Asta*, University of California and Lawrence Berkeley National Laboratory, Berkeley, USA: Dynamics of Grain-Boundary Motion Studied by *in-situ* Electron Microscopy and Molecular Dynamics Simulations (19 July 2012)

*T. Maeshima*, Toyota Central R&D Labs., Inc., Aichi, Japan: Prediction of Liquid Phase Behavior during the Rapid Transient Liquid Phase Bonding Process of Steel using Cementite Filler Metals (19 July 2012)

*N. Wanderka*, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin: Is AlCoCrCuFeNi High Entropy Alloy Suitable for High Temperature Application? Investigations by Transmission Electron Microscopy and Three Dimensional Atom Probe (19 July 2012)

*S. Siebentritt*, University of Luxembourg, Belvaux, Luxembourg: Kesterite - A New Material for Solar Cells (20 July 2012)

*H. Noei*, Ruhr-Universität Bochum: Vibrational Spectroscopic Studies on Metal Oxides and Metal-Organic Frameworks (24 July 2012)

*M. Krzywiecki*, Silesian University of Technology, Gliwice, Poland: Studies of CuPc Ultra-Thin Layers Deposited on Si (111) Substrates (26 July 2012)

*A. Maljusch*, Ruhr-Universität Bochum: Integrated Scanning Kelvin Probe - Scanning Electrochemical Microscopy System: Design, Development and Applications (26 July 2012)

*C. Schön*, Max-Planck-Institut für Festkörperforschung, Stuttgart: Energy Landscapes of Chemical Systems and the Modeling of Chemical Processes (27 July 2012, Colloquium)

*X. Min*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Microstructure-Property Relationship for Ti–Mo β-Titanium Alloys and Fe–Mn–Si Shape Memory Alloys (6 Aug. 2012)

*K. Nakano*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Analysis of the Initiation of Plastic Deformation in Fe-C Alloys (6 Aug. 2012)

*K.A. Padmanabhan*, University of Hyderabad, India: A Mechanism of Deformation for Disordered States of Matter (13 Aug. 2012)

*J.-S. Lee*, Hanyang University-ERICA, Ansan, South Korea: Advances in Processing of Ferrous PM Microcomponents using Nano Powders (17 Aug. 2012)

*M. Morales-Silva,* Lawrence Livermore National Lab, CA, USA: Quantum Monte Carlo Methods (21 Aug. 2012)

*M. Morales-Silva*, Lawrence Livermore National Lab, CA, USA: Application of QMC Methods: High-Pressure Hydrogen (22 Aug. 2012)

*E. Povoden-Karadeniz*, Vienna University of Technology: CALPHAD-Integrated Thermokinetic Simulation of Precipitate Evolution (28 Aug. 2012)

*J. Vogelsang,* SIKA AG, Zürich, Switzerland: Do New Concepts for Corrosion Protection have a Chance? (29 Aug. 2012)

*B.-J. Lee*, POSTECH, South Korea: Multi-Scale, Semi-Empirical Atomistic Approaches for Structural Materials Research (31 Aug. 2012)

*D.J. Jarvis,* New Materials & Energy Research, ESA, The Hague Area, The Netherlands: Metallurgy Europe (3 Sep. 2012)

*M. Scott Shell*, University of California, Santa Barbara, CA, USA: Understanding Peptide Self-Assembly with All-Atom and Coarse-Grained Simulations (3 Sep. 2012)

*S. Lozano-Perez*, Oxford University, UK: High-Resolution Characterisation of Stress Corrosion Cracking in Stainless Steels (7 Sep. 2012)

*M. Ilhan*, Universität Duisburg-Essen: *Ab initio* simulations of the onset of proton mobility in water-starved polymer electrolyte membrane pores (10 Sep. 2012)

*N. Mattern*, IFW Dresden: Phase-Separated Metallic Glasses (11 Sep. 2012)

*A. Stierle*, DESY Nanolaboratory, Hamburg: Oxidation of Alloys and *In-situ* X-Ray Diffraction: Subsurface Superlattice Disordering and the Role of Steps (20 Sep. 2012)

*D. Evans*, University of South Australia, Adelaide, Australia: Thin Film Coatings for Real World Applications: From Conducting Polymers to Transition Metal Alloys (21 Sep. 2012)

*S. Brinckmann*, Ruhr-Universität Bochum: Sequential and Concurrent Multiscale Simulations of Metal Fracture (24 Sep. 2012)

*M. Katsnelson*, Nijmegen University, The Netherlands: Graphene as a Prototype Membrane: Ripples, Puddles and Strain Engineering (2 Oct. 2012)

*A.H. Romero Castro*, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional (Cinvestav) Unidad Querétaro, Mexico: Designing Materials from Scratch: Probing Theoretical Methods (25 Oct. 2012)

*V. Šima*, Charles University Prague, Czech Republic: Recent Experience and Results Obtained with Spark Plasma Sintered FeAl Intermetallics in Prague (6 Nov. 2012)

*M. Spiegel*, Salzgitter Mannesmann Forschung GmbH, Duisburg: Material Requirements for the Energy Transition (6 Nov. 2012, Colloquium)

*S. Neumeier*, Friedrich-Alexander-Universität Erlangen-Nürnberg: $\gamma'$-Hardened Cobalt-Base Superalloys - A New Class of High Temperature Materials (19 Nov. 2012)

*M.J. Cordill*, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences and Montanuniversität Leoben: Mechanical and Interfacial Behavior of Copper and Titanium Films on Polyimide at Elevated Temperatures (20 Nov. 2012, Colloquium)

*S. Curiotto*, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Aix-Marseille University, Marseille, France: Interfacial Morphologies and Orientation Relationships between Copper Crystals and Sapphire (22 Nov. 2012)

# Lectures and Teaching at University

## 2011

*A. Erbe*, Ruhr-Universität Bochum: Physical Chemistry V: Molecular Reaction Dynamics, WS 2011/2012

*T. Hickel*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, compact course, Mar. 2011

*T. Hickel, R. Drautz, J. Neugebauer*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2011/2012

*K.J.J. Mayrhofer,* Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2011 and Part I, WS 2011/2012

*J. Neugebauer*, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2011

*J. Neugebauer*, Ruhr-Universität Bochum: Lecture of the International Max Planck Research School Surmat, Module T3 “Multiscale Modelling”, 2011

*D. Raabe*, RWTH Aachen: Micromechanics of Materials, SS 2011

*M. Rohwerder*, Ruhr-Universität Bochum: Werkstoffoberflächen und Korrosion, SS 2011

*F. Roters*, RWTH Aachen: Process- and Materials Simulation, WS 2011/2012

*F. Roters*: Modellierung von Verformungsvorgängen auf Basis der Kristallplastizität, DGM Fortbildung Modellierung und Simulation, ICAMS Bochum, 18 Nov. 2011

*R. Spatschek, F. Varnik*, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, compact course, May 2011

*R. Spatschek*, Ruhr-Universität Bochum: Stochastic Processes, SS 2011

*R. Spatschek, F. Varnik*, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2011/2012

*S. Zaefferer, T. Hickel and U. Prahl*, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2011

*S. Zaefferer*, University of Vienna, Austria: Fundamentals and applications of texture and EBSD-based orientation microscopy, compact course, Apr. 2011

## 2012

*G. Dehm*, Universität Salzburg: Materialwissenschaften 1, WS 2012/2013

*A. Erbe,* Ruhr-Universität Bochum: Spectroscopy of Surfaces and Interfaces, WS 2012/2013

*T. Hickel, R. Drautz, J. Neugebauer*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2012/2013

*G. Madsen, J. Neugebauer*, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2012

*K.J.J. Mayrhofer,* Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2012 and Part I, WS 2012/2013

*J. Neugebauer*, Ruhr-Universität Bochum: Lecture of the International Max Planck Research School Surmat, Module T3 “Multiscale Modelling”, 2012

*D. Raabe*, RWTH Aachen: Micromechanics of Materials, SS 2012

*M. Rohwerder,* Ruhr-Universität Bochum: Werkstoffoberflächen und Korrosion, SS 2012

*R. Spatschek, F. Varnik*, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2012/2013

*S. Zaefferer, T. Hickel and U. Prahl*, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2012

# Invited Talks at Conferences and Colloquia

## *2010 (not included in Scientific Report 2009/2010)*

Choi, P.: *Characterization of CuInSe$_2$ and CuInGaSe$_2$ thin-film solar cells using atom probe tomography.* (Int. Conf. on Electronic Materials and Nanotechnology for Green Environment (ENGE 2010), Jeju Island, South Korea, 21 to 24 Nov. 2010).

Cojocaru-Mirédin, O.; Choi, P.; Würz, R.; Liu, T.; Raabe, D.: *Characterization of CuInSe$_2$ and Cu(In,Ga)Se$_2$ thin-film solar cells using atom probe tomography.* (Seminar talk at Centre for Solar Energy and Hydrogen Research (ZSW), Stuttgart, Germany, 02 Dec. 2010).

Fabritius, H.; Nikolov, S.; Hild, S.; Ziegler, A.; Friák, M.; Neugebauer, J.; Raabe, D.: *Design principles of arthropod cuticle evaluated experimentally and by ab initio-based multiscale simulations.* (Ringberg Symp. 2010, Molecular Bionics - From Biomineralization to Functional Materials, Ringberg Castle, Tegernsee, Germany, 03 to 06 Oct. 2010).

Freysoldt, C.: *Fully ab initio finite-size corrections for electrostatic artifacts in charged-defect supercell calculations.* (Psi-k Conf. 2010, Berlin, Germany, 12 to 16 Sept. 2010).

Friák, M.; Zhu, L.-F.; Dick, A.; Hickel, T.; Neugebauer, J.: *First-principles study of the Ti–Fe eutectic system.* (Seminar talk at Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 24 Sept. 2010).

Gerstl, S.S.A.: *Instrumentation and software; Reconstruction; Data analyses; Case study of advanced materials.* (Atom Probe Tomography - Workshop Part 4, 52nd Int. Field Emission Symp., University of Sydney, Australia, 05 to 08 July 2010).

Kostka, A.; Springer, H.: *Fundamental research on the role of intermetallic phases in Al-Fe joints.* (Improving Performance and Productivity of Integral Structures through Fundamental Understanding of Metallurgical Reactions in Metallic Joints - VI-IPSUS Summer School, Hamburg, Germany, 30 Aug. to 03 Sept. 2010).

Krüger, T.: *Mesoscopic modeling of red blood cell dynamics.* (Seminar talk on Theory of Complex Systems, Institute for Theoretical Physics, University of Heidelberg, Germany, 16 Dec. 2010).

Mayrhofer, K.J.J.: *The particle-size effect in electrocatalysis.* (Seminar talk at National Institute of Chemistry, Ljubljana, Slovenia, 08 Apr. 2010).

Neugebauer, J.: *Stahldesign in der Wunderwelt der Quantenmechanik.* (Open Day, Stahlzentrum, Düsseldorf, Germany, 04 Sept. 2010).

Neugebauer, J.: *Ab initio based multiscale modeling of advanced electronic, structural and biological materials.* (Colloquium talk at Montan-Universiät Leoben, Austria, 13 Dec 2010).

Raabe, D.; Fabritius, H.; Nikolov, S.; Petrov, M.; Friák, M.; Elstnerová, P.; Neugebauer, J.: *Ab initio based multiscale modeling of biological composites: Example of the exoskeleton of the lobster Homarus americanus.* (Colloquium talk at Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität München, Germany, 09 Nov. 2010).

Raabe, D.; Roters, F.; Dmitrieva, O.; Dick, A.; Hickel, T.; Zaefferer, S.; Ponge, D.; Neugebauer, J.: *Crystal mechanics of the martensitic transformation: crystal plasticity, ab initio models, experiments.* (Colloquium talk at Institute for Mechanics, University of Dortmund, Germany, 18 Nov. 2010).

Raabe, D.; Li, Y.J.; Choi, P.; Dmitrieva, O.; Kirchheim, R.; Ponge, D.: *Towards the limits of strength: Design and understanding of ultra high strength steels.* (Colloquium talk at Ludwig-Maximilians-Universität München, Germany, 19 Nov 2010).

Sandlöbes, S.; Zaefferer, S.: *Effect of RE elements on the deformation and recrystallization behaviour of Magnesium.* (Rare Earth Elements in Magnesium Alloys - MagNET Workshop 5, Vancouver, Canada, 27 to 28 Oct. 2010).

Sandlöbes, S.; Senk, D.: *Automatisierung im Stahlwerk durch in-situ Ab- und Prozessgasmessung.* (8th Aachen Colloquium on Maintenance, Diagnosis and Monitoring System (AKIDA), Aachen, Germany, 17 to 18 Nov. 2010).

Stratmann, M.: *Intelligent corrosion protection by conducting polymer based nanocomposite coatings.* (Gesellschaft Deutscher Chemiker - GDCh Colloquium, Oldenburg, Germany, 25 Nov. 2010).

Todorova, M.: *Corrosion from first principles: A new approach to construct electrochemical E-pH diagrams.* (Crystallographic Colloquium at Ludwig-Maximilians-Universität München, Germany, 29 Oct. 2010).

## *2011*

Auer, A.A.: *Mathematical methods in quantum chemistry.* (Workshop on Mathematical Methods in Quantum Chemistry, Mathematical Research Institute, Oberwolfach, Germany, 26 June to 02 July 2011).

Auinger, M.: *Theory and experiment for high temperature metal-gas reactions.* (Seminar talk at Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, USA, 11 Nov. 2011).

Choi, P.: *Characterization of advanced functional and structural materials using atom probe tomography.* (Inauguration Symp. for the Atom Probe Facilities, Eidgenössische Technische Hochschule Zürich, Switzerland, 06 Dec. 2011).

Choi, P.: *Study of local chemical gradients in advanced precipitation hardened steel using atom probe tomography.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Cojocaru-Mirédin, O.; Choi, P.; Abou-Ras, D.; Würz, R.; Raabe, D.: *Characterization of CI(G)S thin-film solar cells using atom probe tomography.* (37th IEEE Photovoltaic Specialists Conf. (PVSC), Seattle, WA, USA, 19 to 24 June 2011).

Cojocaru-Mirédin, O.; Choi, P.; Würz, R.; Abou-Ras, D.; Raabe, D.: *Explorer les interfaces à l'échelle atomique dans les cellules photovoltaïques CIGSe.* (Seminar talk at Commissariat à l'Energie Atomique et aux Energies Alternatives, Grenoble, France, 05 Dec. 2011).

Eisenlohr, P.; Diehl, M.; Roters, F.; Lebensohn, R.A: *Solving finite-deformation crystal elasto-viscoplasticity with a fast Fourier transformation-based spectral method.* (The Minerals, Metals & Materials Society - TMS Annual Meeting, San Diego, CA, USA, 27 Feb. to 03 Mar. 2011).

Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Roters, F.; Raabe, D.: *A modular crystal plasticity framework applicable from single grain to component scale.* (The Minerals, Metals & Materials Society - TMS Annual Meeting, San Diego, CA, USA, 27 Feb. to 03 Mar. 2011).

Eisenlohr, P.; Roters, F.; Kords, C.; Diehl, M.; Lebensohn, R.A.; Raabe, D.: *Combining characterization and simulation of grain-scale plasticity in three dimensions.* (Electron Back Scattering Diffraction - EBSD Conf. 2011 of the Royal Microscopical Society (RMS), Düsseldorf, Germany, 28 to 30 Mar. 2011).

Eisenlohr, P.; Amberger, D.: *Creep-resistant Mg-alloys - benefits of an intermetallic phase skeleton.* (Materials Engineering Seminar, University of Kassel, Germany, 11 July 2011).

Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Roters, F.; Raabe, D.: *A modular crystal plasticity framework applicable from single grain to component scale.* (XI Int. Conf. Computational Plasticity, Barcelona, Spain, 07 to 09 Sept. 2011).

Erbe, A.: *Thin amorphous oxides and intermediates in chemical reactions: Challenging problems in interface science probed with photons.* (Mini-Workshop on Surface Science for Inauguration of the Turkish Surface Science Society, Ankara, Turkey, 23 May 2011).

Erbe, A.: *Oberflächendesign für empfindliche ATR-Spektroskopie in Modellexperimenten zum Verständnis der Korrosion.* (User meeting - Bruker Optics, Ettlingen, Germany, 22 Nov. 2011).

Fabritius, H.; Nikolov, S.; Hild, S.; Ziegler, A.; Friák, M.; Neugebauer, J.; Raabe, D.: *Mechanical design principles of crustacean cuticle evaluated experimentally and by ab initio-based multiscale simulations.* (Colloquium talk at Institut de Mécanique des Fluides et des Solides (IMFS), Centre national de la recherche scientifique - CNRS, Strasbourg, France, 17 Mar. 2011).

Fabritius, H.; Nikolov, S.; Hild, S.; Ziegler, A.; Friák, M.; Neugebauer, J.; Raabe; D.: *Design principles of crustacean cuticle: From molecules to skeletal elements.* (Workshop „From Nanoparticle Assembly to Functional Polymer Components", Department of Geo- and Environmental Sciences, Ludwig-Maximilians-Universität München, Germany, 08 July 2011).

Freysoldt, C.; Pfanner, G.; Neugebauer, J.: *The dangling-bond defect in amorphous silicon: Insights from theoretical calculations of the EPR parameters.* (Workshop "Advanced EPR for material and solar energy research", Berlin, Germany, 13 to 14 Oct. 2011).

Friák, M.; Zhu, L.-F.; Dick, A.; Udyansky, A.; von Pezold, J.; Emmerich, H.; Neugebauer, J.: *On selected methodological challenges at the interface between quantum-mechanical approaches and phase-field modeling methods in computational materials science*. (Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 14 to 18 Mar. 2011).

Friák, M.; Nikolov, S.; Petrov, M.; Elstnerová, P.; Sachs, C.; Fabritius, H.; Ma, D. ; Lymperakis, L.; Hild, S.; Zigler, A.; Raabe, D.; Neugebauer, J.: *Ab initio based study of multi-scale elastic oproperties of hierarchical biocomposites*. (Multiscale Computational Biomechanics - CECAM Workshop, Zürich, Switzerland, 13 Apr. 2011).

Friák, M.; Nikolov, S.; Petrov, M.; Elstnerová, P.; Sachs, C.; Fabritius, H.; Ma, D.; Lymperakis, L.; Hild, S.; Zigler, A.; Raabe, D.; Neugebauer, J.: *Arthropod cuticle: A biological multi-functional composite used as template for nano-to-macro-scale hierarchical modeling*. (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 04 Aug. 2011).

Gutierrez-Urrutia, I.; Dick, A.; Hickel, T.; Neugebauer, J.; Raabe, D.: *Understanding TWIP steel microstructures by using advanced electron microscopy and ab initio predictions.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Gutierrez-Urrutia, I.; Raabe, D.: *The influence of planar slip and deformation twinning on mechanical behavior in TWIP steels.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Gutierrez-Urrutia, I.; Raabe, D.: *Study of deformation twinning and planar slip in a TWIP steel by electron channelling contrast imaging in a SEM.* (Int. Conf. on the Textures of Materials - ICOTOM 16, Bombay, India, 12 to 17 Dec. 2011).

He, C.; Stein, F.; Palm, M.; Voß, S.: *Thermodynamic assessment of the Fe-Nb and Fe-Al-Nb system.* (3rd Sino-German Symp. on Computational Thermodynamics and Kinetics and their Applications to Solidification and Solid-State Phase Transformation, Xi'an/Shaanxi, China, 20 to 24 June 2011).

Hickel, T.; Körmann, F.; Grabowski, B.; Dick, A.; Neugebauer, J.: *First principles concepts to calculate thermodynamic properties of magnetic materials.* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Advanced Discussions, Ruhr-Universität Bochum, Germany, 10 to 11 Mar. 2011).

Hickel, T.; Grabowski, B.; Körmann, F.; Dick, A.; Neugebauer, J.: *Computational phase studies: Deriving free energies and phase transitions from first principles.* (Centre Européen de Calcul Atomique et Moléculaire - CECAM Workshop 442: Materials Informatics: Tools for Design and Discovery, Lausanne, Switzerland, 23 to 25 May 2011).

Hickel, T.; Grabowski, B.; Nazarov, R.; Sandschneider, N.; Neugebauer, J.: *Ab initio determination of point defects and derived diffusion properties in metals.* (3rd Sino-German Symp., Xi'an/Shaanxi, China, 20 to 25 June 2011).

Hickel, T.: *Ab-initio Modellierung von Stählen.* (Joint Colloquium of the SFB 761 and SFB 799 at Technische Universität Bergakademie, Freiberg, Germany, 05 Sept. 2011).

Hickel, T.; Ismer, L.; Nazarov, R.; von Pezold, J.; Friák, M.; Neugebauer, J.: *Ab initio investigation of hydrogen solubility and mobility in steels: Indentification of hydrogen related mechanisms in steels.* (Steel Hydrogen Conf., Gent, Belgium, 28 to 29 Sept. 2011).

Hickel, T.; Al-Zubi, A.; Neugebauer, J.: *Ab initio based prediction of phase diagrams: Application to magnetic shape-memory alloys.* (9th Materials Day at Ruhr-Universtät Bochum, Germany, 15 Nov. 2011).

Hickel, T.; Glensk, A.; Grabowski, B.; Neugebauer, J.: *Ab initio up to the melting point: Integrated approach to derive accurate thermodynamic data for Al alloys.* (European Aluminium Association, European Aluminium Technology Platform, Working Group 5: Predictive Modelling, 5th Workshop: Ab initio modelling, Aachen, Germany, 01 Dec. 2011).

Jia, N.; Raabe, D.; Zhao, X.: *Experiments and modeling on the development of deformation textures in f.c.c. materials.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Kords, C.; Eisenlohr, P.; Roters, F.; Raabe, D.: *Dislocation flux in three-dimensional crystal plasticity.* (9th Int. Conf. of Numerical Analysis and Applied Mathematics, Halkidiki, Greece, 18 to 25 Sept. 2011).

Kostka, A.; Song, J.; Raabe, D.; Veehmayer, M.: *Explosive cladding of Titanium to low carbon steel: Microstructure and properties.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Mayrhofer, K.J.J.: *IL-TEM for the investigation of nanoparticle corrosion.* (Seminar talk at Rheinische Friedrich-Wilhelms-Universität, Bonn, Germany, 14 Jan. 2011).

Mayrhofer, K.J.J.: *Degradation of carbon-supported fuel cell catalysts.* (Fundamentals and Developments of Fuel Cells - Conf. 2011, Grenoble, France, 19 to 21 Jan. 2011).

Mayrhofer, K.J.J.: *Elektrochemische Hochdurchsatzuntersuchungen mit gekoppelter online Analytik.* (4. Corrosion Protection Symp. - Corrosion protection by coatings in theory and practice, Trent, Rügen, 25 to 27 May 2011).

Mayrhofer, K.J.J.: *Electrocatalysis of PEM fuel cell reactions - Fundamental investigations for real applications.* (9th European Symp. on Electrochem. Engineering, Chania, Greece, 19 to 23 June 2011).

Mayrhofer, K.J.J.: *Catalysis in electrochemical reactors - Fundamental investigations for real applications.* (Seminar talk at Fritz-Haber-Institut of the Max Planck Society (MPG), Berlin, Germany, 22 Aug. 2011).

Mayrhofer, K.J.J.; Hartl, K.; Katsounaros, I.; Meier, J.C.; Hodnik, N.; Arenz, M.: *Activity and stability of Pt-alloy nanoparticles for fuel cell reactions.* (14. Austrian Chemistry Days, Linz, Austria, 26 to 29 Sept. 2011).

Mayrhofer, K.J.J.: *Online investigation of the stability of electrode materials by coupling of SFC-ICP-MS.* (Seminar talk at University of Ulm, Germany, 10 Dec. 2011).

Neugebauer, J.: *Ab initio based modeling of metallic alloys: From a predictive thermodynamic description to tailored mechanical properties.* (Colloquium talk at University of California-Santa Barbara, CA, USA, 23 Feb. 2011).

Neugebauer, J.: *Materials design based on ab initio thermodynamics: Development of accurate and efficient multiscale strategies.* (Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 14 to 18 Mar. 2011).

Neugebauer, J.: *Fully ab initio description of point defect formation and properties at extreme temperatures.* (Materials Research Society - MRS Spring Meeting 2011, San Francisco, CA, USA, 25 to 29 Apr. 2011).

Neugebauer, J.: *Ab initio guided design of materials for photonic applications.* (Colloquium talk at Tyndall University, Cork, Ireland, 10 May 2011).

Neugebauer, J.: *Accuracy and limitations of ab initio approaches in predicting free energies for binaries and unstable phases.* (CALculation of PHAse Diagrams - CALPHAD Workshop, Rio de Janeiro, Brasil, 22 to 27 May 2011).

Neugebauer, J.: *Overview of fundamentals of first principle calculation methods.* (Workshop "From first principles to multi-scale modeling of materials", Pontifícia Universidade Católica do Rio de Janeiro, Department of Engineering Materials, Rio de Janeiro, Brasil, 27 May to 01 June 2011).

Neugebauer, J.: *Ab initio description of alloying effects on extended defects and interfaces.* (Alloying Element Effects on Migrating Interfaces - Alemi Workshop, Vancouver, Canada, 07 to 08 June 2011).

Neugebauer, J.: *Thermodynamic data from first principles: Achievements and challenges.* (Sino-German Symp., Xi'an/Shaanxi, China, 20 to 24 June 2011).

Neugebauer, J.: *Ab initio thermodynamics: From catalytic surfaces to high-strength steels.* (Frontiers in InterfacE Science - Theory And Experiment Symp. - FIESTAE, Berlin, Germany, 29 June to 01 July 2011).

Neugebauer, J.: *Ab initio guided design of materials with superior mechanical properties.* (Colloquium talk at Institute of Technology, Karlsruhe, Germany, 12 July 2011).

Neugebauer, J.: *Ab initio guided materials characterization and design.* (Science Vision for the European Spallation Source (ESS), Bad Reichenhall, Germany, 10 to 12 Oct. 2011).

Neugebauer, J.: *Doping and growth issues in group-III nitrides: An ab initio perspective.* (Workshop on III-Nitrides Growth, Characterization and Simulation, Berlin, Germany, 12 to 13 Oct. 2011).

Neugebauer, J.: *Ab initio based modeling of structural materials with superior properties: From a predictive thermodynamic description to tailored mechanical properties.* (European Congress on Advanced Materials and Processes - EUROMAT 2011, Montpellier, France, 12 to 15 Sept. 2011).

Neugebauer, J.: *Fully ab initio determination of free energies: Methodological challenges and applications.* (Conf. on Computational Physics - CCP2011, Gatlinburg, TN, USA, 30 Oct. to 03 Nov. 2011).

Neugebauer, J.: *Fully ab initio determination of free energies: Achievments and challenges.* (Scientific Group Thermodata Europe - SGTE Workshop, Herzogenrath/Aachen, Germany, 05 to 06 Dec. 2011).

Palm, M.: *Hochleistungswerkstoffe auf Basis intermetallischer Phasen.* (Materials Forum Rhein-Main, Deutsche Gesellschaft für Materialkunde e.V. - DGM, Hanau, Germany, 14 Mar. 2011).

Palm, M.; Krieg, R.: *Neutral salt spray testing on Fe–Al and Fe–Al–X.* (FeAl2011, Discussion Meeting on the Development of Innovative Iron Aluminium Alloys, Lanzarote Canary Islands, Spain, 05 to 07 Oct. 2011).

Pérez-Prado, M.T.; Boehlert, C.; Llorca, J.; Gutiérrez-Urrutia, I.: *In-situ analysis of deformation and recrystallization mechanisms.* (European Congress on Advanced Materials and Processes - EUROMAT 2011, Montpellier, France, 25 to 29 Sept. 2011).

Ponge, D.; Millán, J.; Yuan, L.; Sandlöbes, S.; Kostka, A.; Choi, P.; Hickel, T.; Neugebauer, J.; Raabe, D.: *Nanostructuring of 100 thousand tons.* (Gesellschaft Deutscher Chemiker - GDCh Colloquium, Universität Duisburg-Essen, Essen, Germany, 30 Nov. 2011).

Raabe, D.: *Designing structural metallic materials by combining ab-initio models, atomic scale characterization, and synthesis.* (Colloquium talk at Physics Department, University of Mainz, Germany, 10 May 2011).

Raabe, D.; Ponge, D.: *Alloy design of nanoprecipitate-hardened high-Mn maraging-TRIP.* (The First Int. Conf. on High Manganese Steels, Seoul, South Korea, 15 to 18 May 2011).

Raabe, D.; Roters, F.; Zaefferer, S.; Zambaldi, C.; Demir, E.; Zaafarani, N.; Diehl, M.; Lebensohn, R.A.; Eisenlohr, P.: *Computational crystal plasticity.* (Colloquium talk at Korea Institute of Science and Technology (KIST), Seoul, South Korea, 16 May 2011).

Raabe, D.: *Atomistic understanding of hundred-thousand tons.* (Bernkastel-Kues Workshop "Possibilities and Limitations of Quantitative Materials Modeling and Characterization", Bernkastel-Kues, Germany, 30 May 2011).

Raabe, D.: *Moritaten aus dem Reich der Schmiede: Die Geschichte der Werkstoffe in 45 Minuten.* (Meeting Materials Testing 2011- New developments in materials testing, Berlin, Germany, 01 to 02 Dec. 2011).

Renner, F.U.: *Corrosion behaviour of Fe–Al(–X) alloys in steam.* (Deutsche Gesellschaft für Materialkunde - DGM, Technical Committee Meeting, Technische Universität Dresden, Germany, 08 Feb. 2011).

Renner, F.U.: *Oberflächen auf der atomaren Skala: Entlegierung als ein Beispiel aus der Korrosion.* (Colloquium talk at Technische Universität Hamburg-Harburg, Germany, 08 Sept. 2011).

Rohwerder, M.: *Controlling electronic and ionic mobility in coatings and at interfaces: Novel materials concepts for corrosion protection.* (The Electrochemical Society - 219th ECS Meeting, Montreal, Canada, 01 to 06 May 2011).

Rohwerder, M.: *On the role of micro- and nanostructure of conducting polymers in composite coatings for intelligent corrosion protection.* (The Electrochemical Society - 219th ECS Meeting, Montreal, Canada, 01 to 06 May 2011).

Rohwerder, M.: *Korrosionsschutz durch intelligente release-Systeme.* (4th Corrosion Protection Symp., Rügen, Germany, 25 to 27 May 2011).

Rohwerder, M.: *High-resolution detection of hydrogen: The hydrogen electrode in the dry.* (Simpósio Brasileiro de Eletroquímica e Eletroanalítica - XVIII SIBEEE, Bento Gonçalves-RS, Brazil, 28 Sept. to 01 Oct. 2011).

Rohwerder, M.: *High-resolution detection of hydrogen: The hydrogen electrode in the dry.* (Gesellschaft Deutscher Chemiker - GDCh Colloquium, Greifswald, Germany, 11 Oct. 2011).

Rohwerder, M.: *Scanning Kelvin probe for hydrogen detection with high sensitivity and lateral resolution.* (Seminar talk at Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Dortmund, Germany, 01 Dec. 2011).

Roters, F.; Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Raabe, D.: *A modular crystal plasticity framework applicable from component to single grain scale.* (Int. Union of Theoretical and Applied Mechanics - IUTAM Symp., Linking Scales in Computations: From Microstructure to Macro-scale Properties, Pensacola, FL, USA, 17 to 19 Mar. 2011).

Roters, F.; Tjahjanto, D.D.; C. Kords, C.; Eisenlohr, P.; Raabe, D.: *A modular crystal plasticity framework applicable from component to single grain scale.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 31 July 2011).

Sandlöbes, S.; Friák, M.; Dick, A.; Zaefferer, S.; Pei, Z.; Neugebauer, J.; Raabe, D.: *Combining ab initio calculations and high-resolution experiments to understand advanced Mg alloys.* (German-Korean Workshop on the “Production and industrial applications of semi-finished Mg products”, Irsee, Germany, 02 to 09 Feb. 2011).

Sandlöbes, S.; Friák, M.; Dick, A.; Zaefferer, S.; Pei, Z.; Neugebauer, J.; Raabe, D.: *The effect of rare earth elements on the mechanical properties of Mg - Theory and experiment.* (Rare Earth Elements in Magnesium Alloys - MagNET Workshop 6, Hamilton, Canada, 07 to 08 Nov. 2011).

Spatschek, R.: *Kinetics of phase transitions.* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Advanced Discussions, Ruhr-Universität Bochum, Germany, 10 to 11 Mar. 2011).

Spatschek, R.: *Continuum modeling of metals at high temperatures.* (Seminar „Numerische Mathematik und Mechanik“, Universität Duisburg-Essen, Essen, Germany, 12 Dec. 2011).

Stein, F.: *Fe–Al-based materials: Phase diagrams, properties, and potential for applications.* (Seminar talk at University of Vienna, Austria, 08 Apr. 2011).

Stein, F.: *Experimental determination of phase diagrams as a basis for materials development.* (Seminar talk at University of Nanning, Guangxi, China, 15 Nov. 2011).

Steinmetz, D.; Zaefferer, S.*: Currents state of the art in EBSD: Possibilities and limitations.* (Seminar talk at Ludwig-Maximilians-Universität München, Germany, 06 May 2011).

Stratmann, M.: *Coatings for corrosion protection: An overview of current issues.* (The Electrochemical Society - 220th ECS Meeting, Boston, MA, USA, 09 to 14 Oct 2011).

Todorova, M.: *Stability of polar ZnO(0001) surfaces in dry and humid atmosphere.* (The Thomas Young Centre - TYC Workshop ‘’Thermodynamics and kinetics of dopants, defects and adatoms at surfaces’’, University College London, UK, 22 to 24 June 2011).

Todorova, M.: *Stabilisation of polar ZnO(0001) surfaces in dry and humid environment.* (Theory Seminar at Fritz-Haber-Institut of the Max Planck Society (MPG), Berlin, Germany, 08 Sept. 2011).

Todorova, M.: *Extending the concept of semiconductor defect chemistry to electro-chemistry: Constructing electrochemical E/pH diagrams based on ab-initio calculations.* (Workshop ‘’Modern developments in the ab initio description of charged systems for semiconductors and electrochemistry”, Ringberg Castle, Tegernsee, Germany, 25 Oct. 2011).

von Pezold, J.: *Understanding embrittlement in metals: A multiscale study of the hydrogen enhanced local plasticity (HELP) mechanism.* (Seminar for Materials Research at Max-Planck-Institut für Plasmaforschung, Garching, Germany, 17 Feb. 2011).

Zaefferer, S.: *Diffraction techniques in the scanning electron microscope: Making SEM a universal tool for microstructure research*. (Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 14 Mar 2011).

Zaefferer, S.: *Advanced applications of SEM-based diffraction techniques.* (Int. Union of Microbeam Analysis Societies - IUMAS Conf., Seoul, South Korea, 26 May 2011).

Zaefferer, S.: *Electron diffraction-based techniques in the SEM: Do they give you everything you ever wanted to know about your sample?* (14th Int. Conf. on Emergency Medicine - ICEM 2012, Wisła, Poland, 29 June 2011).

Zaefferer, S.; Jäpel, T.; Tasan, C.; Konijnenberg, P.: *Detailed observation of martensite transformation and twinning in TRIP and TWIP steels using advanced SEM diffraction techniques*. (Int. Conf. on Martensitic Transformations - ICOMAT 2011, Osaka, Japan, 07 Sept. 2011).

Zaefferer, S.: *Comprehensive 5-parameter grain boundary description: How to measure it, how to display it and how important is it?* (Int. Conf. on Martensitic Transformations - ICOTOM 16, Mumbai, India, 15 Nov. 2011).

Zheng, C.W.; Raabe, D.; Li, D.Z.: *Numerical simulation of dynamic strain-induced austenite-ferrite transformation and post-dynamic kinetics in a low carbon steel.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Zhu, L.-F.; Friák, M.; Dick, A.; Hickel, T.; Neugebauer, J.: *Ab initio study of the Ti–Fe eutectic system.* (Erich-Schmid-Colloquium 2011, Erich Schmid Institute of Materials Science (ESI), Austrian Academy of Sciences, Leoben, Austria, 15 Feb. 2011).

## 2012

Albrecht, M.; Markurt, T.; Schulz, T.; Lymperakis, L.; Duff, A.; Neugebauer, J.; Drechsel, P.; Stauss, P.: *Dislocation mechanisms and strain relaxation in the growth of GaN on silicon substrates for solid state lighting* (Conf. on Extended Defects in Semiconductors - EDS 2012, Thessaloniki, Greece, 24 to 29 June 2012).

Auinger, M.: *Experimental studies and theoretical calculations on the formation of nitrides and oxides during selective oxidation in binary iron-alloys.* (8th Int. Symp. on High-Temperature Corrosion and Protection of Materials, Les Embiez, France, 20 to 25 May 2012).

Auinger, M.: *What do we know about internal oxidation in hot-rolled steels? - A theoretical study and its experimental verification.* (Seminar talk at Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany, 09 July 2012).

Auinger, M.: *Internal oxidation and nitridation of hot rolled steels - A theoretical study and its experimental verification.* (Gunnar Eriksson Symp. & GTT, The Single Source for Thermochemistry Tool - Workshop on Thermodynamic Simulations in Industry, Herzogenrath/Aachen, Germany, 11 to 13 July 2012).

Berezkin, A.V.; Biedermann, P.U.: *Multiscale simulation of PU coatings.* (Badische Anilin- & Soda-Fabrik - BASF Seminar, Ludwigshafen, Germany, 24 Apr. 2012).

Chen, Y.; Schneider, P.; Erbe, A.: *Investigation of electrochemical oxide growth on zinc by spectroscopic ellipsometry: An example of in operando spectroscopy.* (Int. Symp. on Electrochem. Micro & Nanosystem Technologies - EMNT 2012 - 9th Int. Symp. on Electrochem. Micro & Nanosystem Technologies, Linz, Austria, 15 to 17 Aug. 2012).

Choi, P.: *Overview of atom probe tomography research at MPIE.* (Material physics seminar at the University of Göttingen, Germany, 09 Feb. 2012).

Choi, P.: *Atom probe characterization of CIGS solar cells.* (Seminar talk at the University of Luxembourg, Luxembourg, 06 Mar. 2012).

Cojocaru-Mirédin, O.; Schwarz, T.; Choi, P.; Würz, R.; Raabe, D.: *Exploring the internal interfaces at the atomic-scale in thin-film solar cells.* (Seminar talk at Helmholtz Zentrum Berlin (HZB), Germany, 25 Mar. 2012).

Cojocaru-Mirédin, O.; Schwarz, T.; Choi, P.; Würz, R.; Abou-Ras, D.; Dietrich, J.; Raabe, D.: *Exploring the internal interfaces at the atomic-scale in* $Cu(In,Ga)Se_2$ *thin-films solar cells.* (1st EU APT Workshop, CEA/MINATEC, Grenoble, France, 04 to 05 Oct. 2012).

Dehm, G.: *In situ micro-mechanical testing at variable temperatures* (12th European Nanomechanical User Group Meeting, University of Malta, 24-25 Oct. 2012).

Dehm, G.: *Prospects and experimental constraints of nano/micro-mechanical testing in materials science* (GDRiCNRS-Mecano General Meeting, Ecole des Mines, Paris, France, 30-31 Oct. 2012).

Dehm, G.; Imrich, P.J.; Kirchlechner, C.; Smolka, M.; Yang, B.; Motz, C.: *In situ micro- and nanomechanical electron microscopy studies of grain boundaries in Cu.* (MRS Fall Meeting 2012, Boston, MA, USA, 25-30 Nov. 2012).

Eisenlohr, P.: *Modeling and simulation of crystal plasticity.* (Chemical Engineering and Materials Science Seminar, Michigan State University, East Lansing, MI, USA, 04 Oct. 2012).

Erbe, A.: *Native and electrochemically grown oxides on metals: The dark side of semiconductor research.* (School for Contacts in Nanosystems Spring Workshop 2012, Niedersächsische Technische Hochschule, Goslar, Germany, 11 May 2012).

Fabritius, H.: *Biologische Verbundwerkstoffe: Korrelation von Struktur, Zusammensetzung und physikalischen Eigenschaften am Beispiel der Arthropodenkutikula.* (Inorganic Chemistry Colloquium, Faculty of Chemistry, Universität Duisburg-Essen, Duisburg, Germany, 17 Apr. 2012).

Friák, M.; Hickel, T.; von Pezold, J.; Zhu, L.-F.; Dick, A.; Counts, W.A.; Sandlöbes, S.; Udyansky, A.; Zaefferer, S.; Roters, F.; Ma, D.; Pei, Z.; Raabe, D.; Holec, D.; Šob, M.; Neugebauer, J.: *Combining ab initio modeling and advanced experimental techniques within multi-scale approaches to materials properties.* (Seminar Talk at Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 24 May 2012).

Friák, M.; Hickel, T.; Abbasi, A.; von Pezold, J.; Zhu, L.-F.; Dick, A.; Sandlöbes, S.; Udyansky, A.; Zaefferer, S.; Ma, D.; Pei, Z.; Raabe, D.; Neugebauer, J.: *Ab initio approaches to stacking fault energy calculations in Mg–Y alloys*. (National Institute for Materials Science - NIMS 2012 Conf., Tsukuba, Japan, 04 to 06 June 2012).

Friák, M.; Ma, D.; Elstnerová, P.; Neugebauer, J.; Raabe, D.; Schindlmayr, A.; Scheffler M.; Šob, M.: *Ab initio study of epitaxy-induced stressed states*. (European Congress on Computational Methods in Applied Sciences and Engineering - ECCOMAS 2012, Vienna, Austria, 10 to 14 Sept. 2012).

Grabowski, B.: *Ab initio prediction of materials properties up to the melting point.* (Seminar series “Condensed Matter and Materials Division”, Lawrence Livermore National Lab, Livermore, CA, USA, 01 Feb. 2012).

Grabowski, B.: *Ab initio prediction of materials properties up to the melting point.* (Seminar “Ab initio Description of Iron and Steel: Thermodynamics and Kinetics”, Ringberg Castle, Tegernsee, Germany, 29 Apr. to 04 May 2012).

Grabowski, B.; Tasan, C.: *SMARTMET project: Towards breaking the inverse ductility-strength relation.* (ThermoCalc Software Workshop, Aachen, Germany, 06 Sept. 2012).

Hafez Haghighat, S.M.; Schäublin, R.: *Atomistic simulation and transmission electron microscopy of obstacle strengthening in iron.* (Seminar talk at Sahand University of Technology, Tabriz, Iran, 01 May 2012).

Hafez Haghighat, S.M.; Eggeler, G.; Raabe, D.: *Dislocation dynamics simulation: methodology and applications.* (Seminar talk at Sahand University of Technology, Tabriz, Iran, 12 May 2012).

Hafez Haghighat, S.M.; Schäublin, R.: *Perspective of multiscale simulation approach in the development of novel materials.* (Seminar talk at Tarbiat Modares University, Tehran, Iran, 19 May 2012).

Hafez Haghighat, S.M.; Eggeler, G.; Raabe, D.: *Primary creep of Ni base supealloys used in hot gas turbine blades.* (Seminar talk at Alstom Company, Baden, Switzerland, 17 Oct. 2012).

Hickel, T.; Dick, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Advancing ab initio to finite temperatures for applications in materials design.* (Spring Meeting of the German Physical Society (DPG), Berlin, Germany, 28 Mar. 2012).

Hickel, T.: *Advancing ab initio methods to finite temperatures: The opening of new routes in materials design.* (Physics Colloquium at Ruhr-Universität Bochum, Germany, 14 May 2012).

Jäpel, T.: *Grundlagen der Kreuzkorrelationsmethode (delta-EBSD): Einführung in CrossCourt3 (CC3) und Erfahrungen in der praktischen Anwendung von CC3.* (Seminar talk at working group EBSD (Electron Backscatter Diffraction), Garbsen, Germany, 04 June 2012).

Janus, A.; Fabritius, H.; Lu, J.; Raabe, D.; Friák, M.; Elstnerová, P.; Neugebauer, J.; Nikolov, S.: *Structural interfaces enable function-related variations of properties in the exoskeleton of crustacea.* (Ringberg Symp. 2012: Generation of Inorganic Functional Materials Implementation of Biomineralization Principles, Ringberg Castle, Tegernsee, Germany, 30 Sept. to 03 Oct. 2012).

Klusemann, B.; Svendsen, B.: *Extended crystal plasticity for dislocation glide and twinning with application to TWIP steels.* (18th Int. Symp. on Plasticity and its Current Applications, San Juan, Puerto Rico, 03 to 08 Jan. 2012).

Klusemann, B.; Svendsen, B.: *Application of non-convex gradient plasticity to the modeling of stress relaxation and microstructure evolution.* (83rd Annual Meeting of the Int. Association for Applied Mathematics and Mechanics (GAMM), Darmstadt, Germany, 26 to 29 Mar. 2012).

Klusemann, B.; Knorr, A.F.; Vehoff, H.; Svendsen, B.: *Experimental investigation and crystal plasticity modeling of sheet metals with coarse texture.* (SEM XII Int. Congress & Exposition on Experimental and Applied Mechanics, Costa Mesa, CA, USA, 11 to 14 June 2012).

Körmann, F.; Dick, A.; Grabowski, B.; Hickel, T.; Neugebauer, J.: *The influence of magnetic excitations on the phase stability of metals and steels.* (Seminar talk at Forschungszentrum Jülich, Germany, 23 May 2012).

Körmann, F.; Grabowski, B.; Hickel, T.; Neugebauer, J.: *Advancing ab initio methods to finite temperatures: The opening of new routes in materials design.* (Seminar talk at Institute on Quantum Materials Science, Yekaterinburg, Russia, 24 June 2012).

Konijnenberg, P.; Khorashadizadeh, A.; Zaefferer, S.; Raabe, D.: *Data mining of 3D EBSD data sets.* (Inauguration of new FIB-SEM instrument at LETAM - Laboratory of Study of Textures and Application to Materials, Metz, France, 13 Dec. 2012).

Kords, C.; Eisenlohr, P.; Roters, F.: *A nonlocal crystal plasticity model used to solve heterogeneous boundary value problems for 3D microstructures.* (18th Int. Symp. on Plasticity & Its Current Applications, San Juan, Puerto Rico, 03 to 08 Jan. 2012).

Kostka, A.; Song, J.; Raabe, D.; Veehmayer, M.: *Structural characterization and analysis of interface formed by explosion cladding of titanium to low carbon steel.* (19th Int. Symp. on Metastable, Amorphous and Nanostructured Materials (ISMANAM), Moscow, Russia, 18 to 22 June 2012).

Liu, B.; Raabe, D.; Eisenlohr, P.; Roters, F.: *Dislocation-hexagonal dislocation network interaction in BCC metals.* (18th Int. Symp. on Plasticity & Its Current Applications, San Juan, Puerto Rico, 03 to 08 Jan. 2012).

Liu, B.; Raabe, D.; Roters, F.: *A dislocation dynamics study of dislocation cell formation and interaction between a low angle grain boundary and in-coming dislocations.* (Partnership for Advanced computing in Europe - 1st PRACE Scientific Conf., Hamburg, Germany, June 2012).

Lymperakis, L.: *Ab initio calculations of energetics, adatom kinetics, and electronic structure of nonpolar and semipolar III-nitride surfaces.* (PolarCoN Summer School, Kloster Kostenz, Konstanz, Germany, 11 to 13 Sept. 2012).

Mayrhofer, K.J.J.: *Stability of electrode materials for clean energy conversion technology.* (American Chemical Society - 243rd ACS National Meeting - ACS Fuel Symp. on Catalysis for Clean Energy Technologies, San Diego, CA, USA, 25 to 29 Mar. 2012).

Mayrhofer, K.J.J.: *Stability of electrode materials for electrochemical energy conversion.* (2nd Ertl Symp. of the Ertl Center for Electrochemistry and Catalysis, Stuttgart, Germany, 24 to 27 June 2012).

Mayrhofer, K.J.J.: *Investigation of electrode material stability for electrochemical energy conversion in fuel cells.* (Seminar talk at National Institute of Chemistry, Ljubljana, Slovenia, 12 July 2012).

Mayrhofer, K.J.J.: *Herausforderungen der Forschung an Elektrokatalysatoren für Niedertemperatur-Brennstoffzellen.* (Materials Science and Engineering - MSE 2012, Darmstadt, Germany, 25 to 27 Sept. 2012).

Mayrhofer, K.J.J.: *Investigation of electrode material durability for electrochemical energy conversion.* (Materials Research Society - 2012 MRS Fall Meeting, Boston, MA, USA, 25 to 30 Nov 2012).

Monas, A.; Spatschek, R.: *Modeling of phase change materials with GPUs.* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Advanced Discussions, Ruhr-Universität Bochum, Germany, 26 to 27 Apr. 2012).

Neugebauer, J.: *Ab initio guided materials design: Concepts, prospects and challenges.* (Seminar talk at University of Münster, Germany, 12 Jan. 2012).

Neugebauer, J.: *Fully ab initio determination of free energies: Application to modern high-strength steels.* (Mini2012 Workshop, Barcelona, Spain, 14 Jan. 2012).

Neugebauer, J.: *Fully ab initio determination of free energies: Where do we stand?* (The Minerals, Metals & Materials Society - TMS Spring Meeting, Orlando, FL, USA, 11 to 15 Mar. 2012).

Neugebauer, J.: *Long time scale simulations to determine accurate ab initio free energies.* (Beyond Molecular Dynamics - BEMOD Workshop, Dresden, Germany, 26 to 29 Mar. 2012).

Neugebauer, J.: *Ab initio guided materials design: Concepts, prospects and challenges.* (Seminar talk at Universität Duisburg-Essen, Duisburg, Germany, 25 Apr. 2012).

Neugebauer, J.: *Electric fields, surfaces and adatom kinetics from an ab initio perspective.* (Int. Field Emission Symp. - IFES 2012, Birmingham, AL, USA, 25 Apr. 2012).

Neugebauer, J.: *Ab initio thermodynamics: Status and perspectives.* (Workshop at State Key Laboratory of Powder Metallurgy, Central South University, Changsha, China, 29 May 2012).

*Neugebauer, J.: Ab initio guided materials design: Concepts, prospects and challenges.* (Seminar talk at Johannes Kepler Universität, Linz, Austria, 31 May 2012).

*Neugebauer, J.: Vacancy concentrations from 0K to the melting temperature in unary fcc metals: Discovery of large non-Arrhenius effects.* (CALculation of PHAse Diagrams - CALPHAD 2012 Meeting, Berkeley, CA, USA, 03 to 08 June 2012).

Neugebauer, J.: *Density functional theory: From the chemical bond to microstructural information.* (Multiscale Materials Modeling 2012 Workshop, Bad Herrenalb, Germany, 02 to 07 Sept. 2012).

Neugebauer, J.: *Fully ab initio determination of materials properties at finite temperatures.* (Electron Correlations and Materials Properties of Compounds and Alloys - ECMPCA 2012, Porto Heli, Greece, 07 to 13 Sept. 2012).

Neugebauer, J.: *Understanding H-embrittlement in high-strength steels by ab initio methods.* (2012 Int. Hydrogen Conf., Moran, WY, USA, 09 to 12 Sept. 2009).

Neugebauer, J.: *Ab initio computation of free energies.* (MDWS1: Workshop on Quantum and Atomistic Modeling of Materials Defects, Los Angeles, CA, USA, 01 to 05 Oct. 2012).

Neugebauer, J.: *Materials design based on ab initio thermodynamics.* (Harnessing the Materials Genome 2012, Vail, CO, USA, 01 to 05 Oct. 2012).

Neugebauer, J.: *Ab initio based multiscale modeling of structural materials: From a predictive thermodynamic description to tailored mechanical properties.* (MMM 2012 - 6th Int. Conf. on Multiscale Materials Modeling, Biopolis, Singapore, Singapore, 15 to 19 Oct. 2012).

Neugebauer, J.; Grabowski, B.; Koermann, F.; Friak, M.; Hickel, T.: *Fully ab initio determination of free energies: Basis for inverse approaches in materials design.* (Materials Research Society - MRS Fall Meeting, Boston, MA, USA, 25 to 30 Nov. 2012).

Neugebauer, J.: *Materials design based on predictive ab initio Thermodynamics.* (Colloquium talk at Imperial College London, UK, 03 to 04 Dec. 2012)

Ponge, D.; Millán, J.; Yuan, L.; Sandlöbes, S.; Kostka, A.; Choi, P.; Hickel, T.; Wittig, J.; Inden, G.; Assadi, H.; Kirchheim, R.; Neugebauer, J.; Raabe, D.: *Nanostructuring of 1 Mio tons: Designing ultrastrong and ductile steels.* (Spring Meeting of the German Physical Society (DPG), Berlin, Germany, 28 Mar. 2012).

Ponge, D.; Millán, J.; Yuan, L.; Zaefferer, S.; P. Konijnenberg, J.; Khorashadizadeh, A.; Sandlöbes, S.; Gutiérrez-Urrutia, I.; Kostka, A.; Choi, P.; Hickel, T.; Neugebauer, J.; Raabe, D.: *The art of experimentation in micromechanics: Lattice defects in steels.* (Int. Association for Applied Mathematics and Mechanics - GAMM Conf., Darmstadt, Germany, 29 Mar. 2012).

Ponge, D.; Millán, J.; Yuan, L.; Sandlöbes, S.; Kostka, A.; Choi, P.; Zaefferer, S.; Hickel, T.; Inden, G.; Assadi, H.; Kirchheim, H.; Neugebauer, J.; Raabe, D.: *Microstructure hierarchy and nanoscale transformations in steels.* (Workshop "Mathematical challenges of materials science and condensed matter physics: From quantum mechanics through statistical mechanics to nonlinear pde", Hausdorff Research Institute for Mathematics, Bonn, Germany, 07 May 2012).

Povstugar, I.; Choi, P.; Tytko, D.; Raabe, D.: *Atom probe tomography for nanoscale analysis of nitride thin films.* (7th Int. Conf. on Surfaces, Coatings and Nanostructured Materials - NANOSMAT 2012, Prague, Czech Republic, 18 to 21 Sept. 2012).

Raabe, D.; Ponge, D.; Choi, P.; Zaefferer, S.; Hickel, T.; Friák, M.; Neugebauer, J.: *Nanostructuring of 1 Million tons: Designing steels using quantum mechanics and atom probe tomography.* (Seminar talk at University of Saarland, Saarbrücken, Germany, 07 Feb. 2012).

Raabe, D.; Millán, J.; Dmitrieva, O.; Ponge, D.; Choi, P.; Inden, G.; Wittig, J.: *Partitioning and austenite reversion at martensite-austenite interfaces in Mn-steels.* (The Minerals, Metals & Materials Society - TMS 2012 Annual Meeting, Orlando, FL, USA, 13 Mar. 2012).

Raabe, D*.: Nanostructures in 1 Billion Tons: Using ab-initio based multiscale models and atomic scale experiments for understanding the mechanical behavior of metallic and biological structural materials.* (Colloquium presentation at Physical Faculty, University of Bremen, Germany, 24 May 2012).

Raabe, D.; Ponge, D.; Choi, P.; Millán, J.; Sandlöbes, S.; Hickel, T.; Neugebauer, J.: *Nanoscale austenite reversion in martensitic and maraging-TRIP steels.* (Plenary talk at 3rd Int. Symp. on Steel Science, Kyoto, Japan, 29 May 2012).

Raabe, D.; Ponge, D.; Choi, P.; Millán, J.; Sandlöbes, S.; Yuan, L.; Tasan, C.; Plancher, E.; Zaefferer, S.; Hickel, T.; Friák, M.; Dick, A.; Inden, G.; Neugebauer, J.: *Designing nanostructured metallic bulk alloys via first principles simulations and atomic scale characterization: The basis of modern manufacturing.* (Plenary talk at National Institute for Materials Science - NIMS 2012 Conf., Tsukuba, Japan, 04 June 2012).

Raabe, D.: *Understanding structure and mechanical properties of the arthropod cuticle using multiscale simulation: Example of Homarus Americanus.* (Plenary talk at Multiscale Materials Modeling - MMM 2012 Conf., Singapore, Singapore, 15 to 19 Oct. 2012).

Ram, F.: *EBSD projection centre's importance and available methods for resolving it!* (Seminar talk at Working Group EBSD (Electron Back Scattering Diffraction), Garbsen, Germany, 04 June 2012).

Renner, F.U.: *Corrosion of model alloys: Binary noble metal alloys and amorphous steel.* (Seminar talk at University of Gießen, Germany, 21 Apr. 2012).

Renner, F.U.: *From inhibition of dealloying to passivation of amorphous steel.* (Seminar talk at University of Ulm, Germany, 12 June 2012).

Renner, F.U.: *Lithium-Ion batteries: Mechanism, material aspects, and challenges.* (Colloquium talk at University of Hasselt, Belgium, 14 June 2012).

Renner, F.U.: *Mesoporous structures by selective dissolution of alloys.* (Int. Symp. on Novel and Nano Materials 2012, Istanbul, Turkey, 26 to 30 Aug. 2012).

Renner, F.U.: *Reaktive Grenzflächen auf der atomaren Skala.* (Colloquium talk at University of Siegen, Germany, 11 Sept. 2012).

Renner, F.U.: *Amorphous steel: Microstructure, corrosion, and surface analysis.* (High Nitrogen Steels & Interstitual Alloys (HNS - 2012), Chennai, India, 27 to 29 Sept. 2012).

Renner, F.U.: *From corrosion to batteries: Studies on electrochemical interfaces.* (Seminar talk at SLAC (National Accelerator Laboratory), Stanford, CA, USA, 18 Oct. 2012).

Rohwerder, M.: *Intelligent corrosion protection: Self-healing concepts based on novel composite coatings.* (Seminar talk at departamento de Ingeniería Hidráulica y Ambiental, Departamento de Ingeniería Mecánica y Metalúrgica, Pontificia Universidad Católica de Chile, Santiago de Chile, Chile, 28 Mar. 2012).

Rohwerder, M.: *High-sensitive and locally resolved hydrogen detection in metals by scanning Kelvin probe technique.* (National Institute for Materials Science - NIMS 2012 Conf., Tsukuba, Japan, 04 to 06 June 2012).

Rohwerder, M.: *Selbstheilende Beschichtungen für einen intelligenten Korrosionsschutz.* („Farbe und Lack“ Conference: New concepts for anti-corrosion coatings, Stuttgart, Germany, 12 to 13 June 2012).

Rohwerder, M.: *High-sensitive and spatially resolved detection of diffusible hydrogen in steels by scanning Kelvin probe microscopy.* (MPIE Workshop on Hydrogen Embrittlement in Steels, Düsseldorf, Germany, 25 June 2012).

Roters, F.; Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Diehl, M.; Raabe, D.: *DAMASK: The Düsseldorf Advanced Material Simulation Kit for studying crystal plasticity using FEM and FFT based numerical solvers.* (18th Int. Symp. on Plasticity & Its Current Applications, San Juan, Puerto Rico, 03 to 08 Jan. 2012).

Roters, F.; Eisenlohr, P.; Diehl, M.; Kords, C.; Raabe, D.: *The general crystal plasticity framework DAMASK.* (Seminar talk at Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany, 16 Apr. 2012).

Roters, F.; Eisenlohr, P.; Diehl, M.; Kords, C.; Raabe, D.: *The general crystal plasticity framework DAMASK.* (Colloquium “Materials Modelling”, Institute for Materials Testing, Materials Science and Strength of Materials (IMWF), Stuttgart, Germany, 14 June 2012).

Sandlöbes, S.; Friák, M.; Pei, Z.; Zaefferer, S.; Yi, S.; Neugebauer, J.; Raabe, D.: *Joint DFT and TEM study on the ductilizing effect of rare earth elements (RE) on Mg alloys.* (The Minerals, Metals & Materials Society - TMS 2012 Annual Meeting, Orlando, FL, USA, 12 Mar. 2012).

Sandlöbes, S.; Friák, M.; Dick, A.; Zaefferer, S.; Pei, Z.; Zhu, L.-F.; Sha, G.; Ringer, S.; Neugebauer, J.; Raabe, D.: *Combining ab initio calculations and high resolution experiments to improve the understanding of advanced Mg–Y and Mg–RE alloys.* (7th Annual Conf. of the Australian Research Council - ARC, Centre of Excellence for Design in Light Metals, Melbourne, Australia, 12 to 14 Nov. 2012).

Schulz, T.; Remmele, T.; Markurt, T.; Korytov, M.; Albrecht, M.; Duff, A.; Lymperakis, L.; Neugebauer, J.: *Alloy fluctuations in III-nitrides revisited by aberration corrected transmission electron microscopy.* (Int. Workshop on Nitride Semiconductors, Sapporo, Japan, 14 to 19 Nov. 2012).

Spatschek, R.: *Kinetics of phase transitions.* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Advanced Discussions, Ruhr-Universität Bochum, Germany, 26 to 27 Apr. 2012).

Stein, F.; Voß, S.; Palm, M.: *Mechanical properties of transition-metal Laves phases.* (Plasticity 2012, Symp. on Plasticity and Its Current Applications, San Juan, Puerto Rico, 03 to 08 Jan. 2012).

Stein, F.: *Laves phases in binary and ternary systems: Stability, structure and mechanical properties.* (Seminar talk at Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany, 24 Apr. 2012).

Stein, F.: *Liquidus surfaces and their relevance for materials development.* (Seminar talk at University of Nanning, Guangxi, China, 18 Sept. 2012).

Stratmann, M.: *Electrocatalysis: How to answer major questions in fundamental research.* (Closing Symp. of the Collaborative Research Centre SFB 558 “Metal-substrate interactions in heterogeneous catalysis”: 2000-2012, Ruhr-Universität Bochum, Germany, 16 to 18 Apr. 2012).

Stratmann, M.: *Electrochemistry: Rebirth of a science.* (Physics Colloquium at Institute of Experimental Physics, University of Innsbruck and Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Innsbruck, Austria, 14 May 2012).

Stratmann, M.: *Coatings for corrosion protection: An overview of current issues.* (Seminar talk at BASF Coatings GmbH, Münster, Germany, 23 July 2012).

Svendsen, B.: *Modeling and characterization of deformation behavior and microstructures in TWIP steels.* (Colloquium for Materials Modeling, Institute for Materials Testing, Materials Science and Strength of Materials (IMWF), University of Stuttgart, Germany, 02 Feb. 2012).

Svendsen, B.: *Material characterization and modeling of the deformation behavior of TWIP steels.* (Seminar talk at Winter School of the Deutsche Forschungsgemeinschaft (DFG), Research Training Group 1483, Karlsruhe Institute of Technology (KIT), Germany, 08 Mar. 2012).

Svendsen, B.: *Thermodynamic variational formulation of dislocation field theory at large deformation.* (Int. Mechanics of Materials Workshop, Mathematical Research Institute, Oberwolfach, Germany, 19 to 24 Mar. 2012).

Svendsen, B.: *On non-local and semi-discrete generalization of continuum dislocation field theory.* (Mini Symp. on Homogenization from Submicro to Micro Scales, 83rd Annual Meeting of the Int. Association for Applied Mathematics and Mechanics (GAMM), Darmstadt, Germany, 26 to 30 Mar. 2012).

Svendsen, B.; Klusemann, B.; Yalcinkaya, T.; Geers, M.: *Modeling of inelastic microstructure development and inhomogeneous material behavior via non-convex rate-dependent gradient plasticity.* (The Chinese Society of Theoretical and Applied Mechanics - XXIII ICTAM, Beijing, China, 19 to 24 Aug. 2012).

Svendsen, B.: *Statistical and mesoscopic approaches to the modeling of collective dislocation behavior.* (Summer School on Multiscale Materials Modeling, Int. Association for Applied Mathematics and Mechanics (GAMM), Karlsruhe Institute of Technology (KIT), Germany, 03 to 07 Sept. 2012).

Svendsen, B.; Hütter, M.: *Application of generic-based coarse-graining methods to the formulation of models for collective dislocation behavior.* (MMM 2012 - 6th Int. Conf. on Multiscale Materials Modeling, Biopolis, Singapore, 15 to 19 Oct. 2012).

Svendsen, B.: *Statistical thermodynamic and mesoscopic formulation of models for collective dislocation behavior.* (1st Int. Workshop on Physics Based Modeling of Materials Properties and Experimental Observations, organized by JRC European Commission, Ankara, Turkey, 22 to 23 Oct. 2012).

Todorova, M.: *Combining ab initio calculations with thermodynamic concepts to address questions related to aqueous corrosion.* (Seminar talk at Department of Theoretical Chemistry, Technische Universität München, Germany, 07 Feb. 2012).

Todorova, M.: *Extending the concept of semiconductor defect chemistry to electro-chemistry: Potential and challenges.* (Seminar talk at Department of Theoretical Chemistry, Universität Duisburg-Essen, Essen, Germany, 16 Feb. 2012).

Todorova, M.: *Extending thermodynamic concepts combined with first-principles calculations to address questions related to aqueous corrosion: Potential and challenges.* (Seminar talk at Department of Theoretical Chemistry, University of Ulm, Germany, 17 July 2012).

Todorova, M.: *Extending the concept of semiconductor defect chemistry to electro-chemistry.* (CMD-24/ECOSS-29/ECS (The Electrochemical Society), CD-11/CMMP-12, Edinburgh, UK, 03 to 07 Sept. 2012).

Valtiner, M.: *The electrochemical surface force apparatus: From surface forces to nanoscale real-time imaging of electrochemical reactions at confined interfaces.* (Gordon Research Conf.: Corrosion - Aqueous, New London, NH, USA, 08 to 13 July 2012).

Zaefferer, S.; Chen, J.; Konijnenberg, P.: *A study on origin and nature of shear bands in cold rolled Mg-3Y alloy using 3D EBSD.* 11.07.2012, (9th Int. Conf. on Magnesium Alloys and their Applications, Vancouver, Canada, 11 Feb. 2012).

Zaefferer, S.: *Dislocations in metals: Observations from the atomic scale to macroscopic dimensions.* (Institute for Complex Molecular Systems - ICMS Workshop “Open problems between micro and macro systems of agents and particles”, University of Technology, Eindhoven, The Netherlands, 19 Apr. 2012).

Zaefferer, S.: *Advanced applications of SEM-based electron diffraction techniques for the characterization of deformation structures of new steels.* (European Materials Research Society - E-MRS 2012, Strasbourg, France, 26 May 2012).

Zaefferer, S.: *An overview on techniques for the measurements of plastic and elastic strain by EBSD and related techniques.* (Electron Back Scattering Diffraction - EBSD User Meeting of the DGK (Deutschen Gesellschaft für Kristallographie), Hannover, Germany, 04 June 2012).

Zaefferer, S.; Konijnenberg, P.; Khorashadizadeh, A.; Chen, J.: *Advanced analysis of 3D EBSD data obtained from FIB-EBSD tomography.* (Microscopy & Microanalysis 2012, Phoenix, AZ, USA, 01 Aug. 2012).

Zaefferer, S.: *Application of advanced diffraction techniques in the SEM.* (European Microscopy Congress - EMC 2012, Manchester, UK, 19 Sept. 2012).

Zaefferer, S.: *Advanced applications of SEM-based electron diffraction techniques.* (2nd EDAX EBSD User Meeting, Wiesbaden, Germany, 21 Nov. 2012).

Zambaldi, C.; Yang, Y.; Bieler, T.R.; Raabe, D.: *Bestimmung der Einkristallplastizität von Titan durch orientierungsabhängige Indentierung.* (Seminar talk at Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany, 22 June 2012).

Ziegler, A.; Ruangchaj, S.; Seidl B.; Huber, J.; Hild, S.; Reisecker, C.; Raabe, D.; Fabritius, H.; Janus, A.; Karsten, S.; Lu, J.; Neugebauer, J.; Friák, M.; Elstnerová, P.; Nikolov, S.: *Crustacean skeletal elements: Variations in the constructional morphology at different hierarchical levels.* (DFG (Deutsche Forschungsgemeinschaft) Winter School of the Priority Programme 1420: “Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials”, Potsdam, Germany, 19 to 20 Mar. 2012).

# Publications

## 2010 (not included in Scientific Report 2009/2010)

### Publications in Scientific Journals

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# Habilitation, Doctoral, Diploma, Master and Bachelor Theses

## Habilitation Theses

### 2011

*PD Dr. F. Roters:* Advanced material models for the crystal plasticity finite element method - Development of a general CPFEM framework (RWTH Aachen)

## Doctoral Theses

### 2010 (not included in Scientific Report 2009-2010)

*Dr.-Ing. M. Calcagnotto:* Ultrafine grained dual-phase steels (RWTH Aachen)

*Dr.rer.nat. F.R. Hamou:* Numerical investigation of scanning electrochemical potential microscopy (SECPM) (Ruhr-Universität Bochum)

*Dr.rer.nat. A. Laaboudi:* Sauerstoffreduktion auf Thiol-modifizierten Au(111)-Oberflächen (Ruhr-Universität Bochum)

*Dr.-Ing. Ö. Özlem:* Synthesis, characterisation and functionalisation of ZnO nanorods on metals (Ruhr-Universität Bochum)

### 2011

*Dr.-Ing. G.N. Ankah:* Investigations of the selective dissolution of $Cu_3Au(111)$: *In-situ* and *ex-situ* Characterization (Ruhr-Universität Bochum)

*Dr.phil. B. Britton:* Measurement of residual elastic strain and lattice rotations with high resolution electron backscatter diffraction (Oxford University, UK)

*Dr.rer.nat. A. Karschin:* Liganden-stabilisierte Rhodium-Nanocluster (Heinrich-Heine-Universität Düsseldorf)

*Dr.-Ing. T.R. Khan:* Nanocomposite coating: Codeposition of $SiO_2$ particles during electrogalvanizing (Ruhr-Universität Bochum)

*Dr.-Ing. A. Khorashadizadeh:* Microstructure characterization of ultra-fine grained Cu−0.17wt.%Zr (RWTH Aachen)

*Dr.rer.nat. S.O. Klemm:* Microelectrochemical characterization of Zn, ZnO and Zn−Mg alloys with online dissolution monitoring (Ruhr-Universität Bochum)

*Dr.rer.nat. F. Körmann*: Magnetic systems studied by first-principles thermodynamics (Universität Paderborn)

*Dr.rer.nat. T. Krüger:* Computer simulation study of collective phenomena in dense suspensions of red blood cells under shear (Ruhr-Universität Bochum)

*Dr.-Ing. Y. Lü:* Deformation and recrystallization behaviour of Fe−Mn−C alloys (RWTH Aachen)

*Dr.-Ing. D. Ma:* First-principles investigations of solid solution strengthening in Al alloys (RWTH Aachen)

*Dr.-Ing. B. Özkaya:* Molecular adsorption studies at heterogeneous oxide/electrolyte interface (Ruhr-Universität Bochum)

*Dr.rer.nat. M. Reithmeier:* Antireflecting Interlayers for enhancing transparency of metal layers for internal reflection infrared wpectroscopy (Ruhr-Universität Bochum)

*Dr.-Ing. A. Saeed-Akbar:* Mechanism maps, mechanical properties, and flow behavior in high-manganese TRIP / TWIP and TWIP steels (RWTH Aachen)

*Dr.-Ing. C. Senöz:* High resolution investigation of localized corrosion by *in-situ* SKPFM (Ruhr-Universität Bochum)

*Dr.-Ing. J. Song:* Microstructure and properties of interfaces formed by explosion cladding of titanium to low carbon steel (Ruhr-Universität Bochum)

*Dr.-Ing. H. Springer:* Fundamental research into the role of intermetallic phases in joining of aluminium alloys to steel (Ruhr-Universität Bochum)

*Dr.-Ing. S. Voß:* Mechanische Eigenschaften von Laves-Phasen in Abhängigkeit von Kristallstruktur und Zusammensetzung am Beispiel der Systeme Fe−Nb−Al und Co−Nb (RWTH Aachen)

### *2012*

*Dr.rer.nat. S. Borodin:* Präparation und Charakterisierung von Metalloxidoberflächen für grundlegende Untersuchungen der Selbstorganisation von Phosphonsäuren (Ruhr-Universität Bochum)

*Dr.-Ing. T. Colding Lomholt*: Microstructure evolution during friction stir spot welding of TRIP steel (Technical University of Denmark, Copenhagen, Denmark)

*Dr.-Ing. M. Dumont:* Hierarchical structure and diagenesis of sauropod long bones using advanced characterization techniques (University of Bonn)

*Dr.rer.nat. M. Gross:* Thermal fluctuations in non-ideal fluids with the Lattice Boltzmann method (Ruhr-Universität Bochum)

*Dr.-Ing. C. Hostert:* Towards designing elastic and magnetic properties of Co-based thin film metallic glasses (RWTH Aachen)

*Dr.rer.nat. B. Lange*: Limitierungen der p-Dotierbarkeit von Galliumnitrid (Universität Paderborn)

*Dr.-Ing. B. Liu:* Discrete dislocation dynamics simulations of dislocation-low angle grain boundary interactions (RWTH Aachen)

*Dr.rer.nat. N. Moradi:* Lattice Boltzmann simulation of droplet dynamics on solid surfaces (Ruhr-Universität Bochum)

*Dr.-Ing. M.I. Muglali:* Pyridine-functionalized araliphatic organothiol films on Au: Surface engineering and characterization (Ruhr-Universität Bochum)

*Dr.rer.nat. G. Pfanner*: The dangling-bond defect in silicon: Insights into electronic and structural effects from first-principles calculations of the EPR-parameters (Universität Paderborn)

*Dr.-Ing. G. Vasan:* Numerical investigation of rough model surfaces in attenuated total reflection surface enhanced infrared absorption spectroscopy with correlating experiments (Ruhr-Universität, Bochum)

*Dr.rer.nat. H. Venzlaff:* Die elektrisch mikrobiell beeinflusste Korrosion von Eisen durch sulfatreduzierte Bakterien (Ruhr-Universität Bochum)

*Dr.-Ing. L. Yuan:* Nanoscale austenite reversion through partitioning, segregation and kinetic freezing (RWTH Aachen)

## Diploma Theses

### *2010 (not included in Scientific Report 2009-2010)*

*M. Diehl:* A spectral method using fast Fourier transform to solve elastoviscoplastic mechanical boundary value problems (TU München)

*K. Hausmann*: Cementite in ferrite from first-principles: Influence of substitutional impurities on thermodynamic stability (RWTH Aachen)

### *2011*

*M. Belde:* Microtexture of NiW during recrystallization - Textured substrate for HT superconductors (RWTH Aachen)

*T. Schwarz:* Lumineszenzuntersuchungen von Cu(In,Ga)$Se_2$-Dünnschichtsolarzellen (Otto-von-Guericke-Universität Magdeburg)

*R. Schulz*: Mesoskalen-Modellierung von pine tree nanowires (Ruhr-Universität Bochum)

### *2012*

*K.-D. Bauer*: Modeling liquid metal embrittlement (Johannes-Kepler-Universität Linz, Austria)

*J. Nellessen*: Dehnratenabhängiges Fließ- und Umwandlungsverhalten hoch-manganhaltiger TWIP-Stähle (RWTH Aachen)

*Z. Pei*: Understanding the impact of solutes on the ductility of magnesium: An *ab initio* study (RWTH Aachen)

## Master Theses

### *2010 (not included in Scientific Report 2009-2010)*

*N. Hamidi Siboni:* Statistical and quantum mechanical simulation of interstitials in metals: Mechanisms and constraints for superabundant vacancy formation (RWTH Aachen)

### *2011*

*J. Chen:* Characterization of the nature of shear bands and deformation bands in cold rolled Mg−Y alloys using 3D and high angular resolution EBSD techniques (RWTH Aachen)

*J. Chu:* Fe−Cr−Mo alloys design: Application to dental alloy and metallic glass (RWTH Aachen)

*C. Du:* Atom probe characterization of single crystalline superalloys (RWTH Aachen)

*H. Hu:* Thermal stability of hard coatings studied by atom probe tomography (RWTH Aachen)

*Y. Ievskaya:* Analysis of dissipative heating in crystal plasticity at the grain scale (RWTH Aachen)

*J. Lu:* Correlation of microstructure, composition and mechanical properties to function in the mandibles of arthropoda (RWTH Aachen)

*E. Plancher:* Strain measurement by high resolution EBSD (Ecole des mines de Saint-Etienne/EDF, France)

*R. Seeger:* Analysis of the subsurface microstructure of metal/metal hip joints by means of TEM and atom probe tomography (University of Duisburg-Essen, Duisburg)

*Y. Wang:* Comparative study of deformation and recrystallization mechanisms of $Mg_{97}Zn_1Y_2$ and $MgY_3$ at elevated temperatures (RWTH Aachen)

### *2012*

*N. Buller*: Untersuchung der elektrochemischen reduktiven Desorption von Thiolen auf Goldelektroden mit spektroskopischer Ellipsometrie (Carl von Ossietzky Universität Oldenburg)

*D. Hessling:* Probing the interaction of grain boundaries and dislocation slip by nanoindentation (FH Düsseldorf)

*D. Korbmacher*: Dual scale modeling of hydrogen embrittlement (Ruhr-Universität Bochum)

*M. Kuzmina:* Study of equilibrium segregation of Mn and reversion of austenite in tempered medium manganese steels and its influence on impact toughness (RWTH Aachen)

*A. Monas*: Modeling of phase change materials for nonvolatile data storage using GPU simulations (Ruhr-Universität Bochum)

*S. Qin:* Experimental investigation on the relationship of grain boundary character and local carbon partitioning in a quench-and-partitioning (QP) steel (RWTH Aachen)

*N. Tillack:* Chemical Trends in the yttrium-oxide precipitates in oxide dispersion strengthened steels: A first-principles investigation (Ruhr-Universität Bochum)

*M. Wang:* Strain hardening behavior of high-Mn steels (RWTH Aachen)

*J. Wang*: Austenite reversion in 0.45C-13.5Cr martensitic stainless steels: Influence of Mn concentration and tempering conditions on the evolution of microstructure and mechanical properties (RWTH Aachen)

*D. Yan:* Determination of mechanical values and flow curves of high strength steels for automotive seat parts after painting process (RWTH Aachen)

*J. Zhang:* An approach to measure residual stress in TWIP steels using nanoindentation (RWTH Aachen)

## Bachelor Thesis

### *2011*

*D. Korbmacher:* Entwicklung von Kontinuumsmodellen zur Wasserstoffversprödung an Rissen (Ruhr-Universität Bochum)

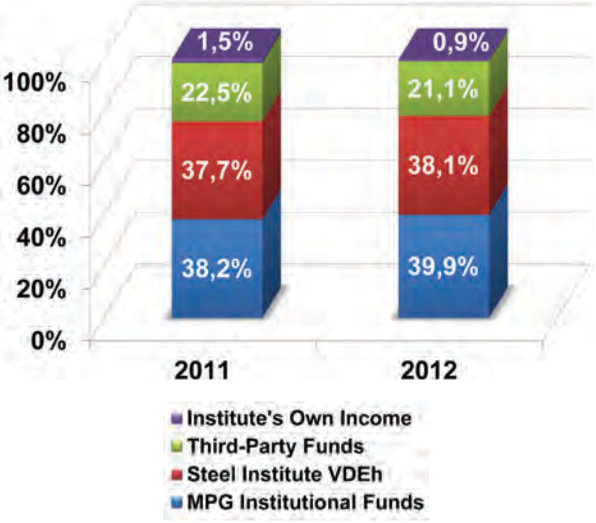
### *2012*

*F. Twiste*: Untersuchung von Schmelzprozessen entlang von Korngrenzen mittels Greensfunktionsmethoden (Heinrich-Heine-Universität Düsseldorf)

# Budget of the Institute

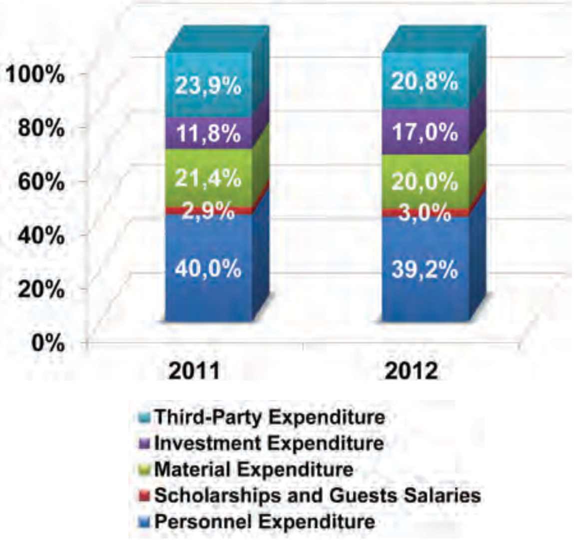
## Revenue

(percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2012 data estimated)



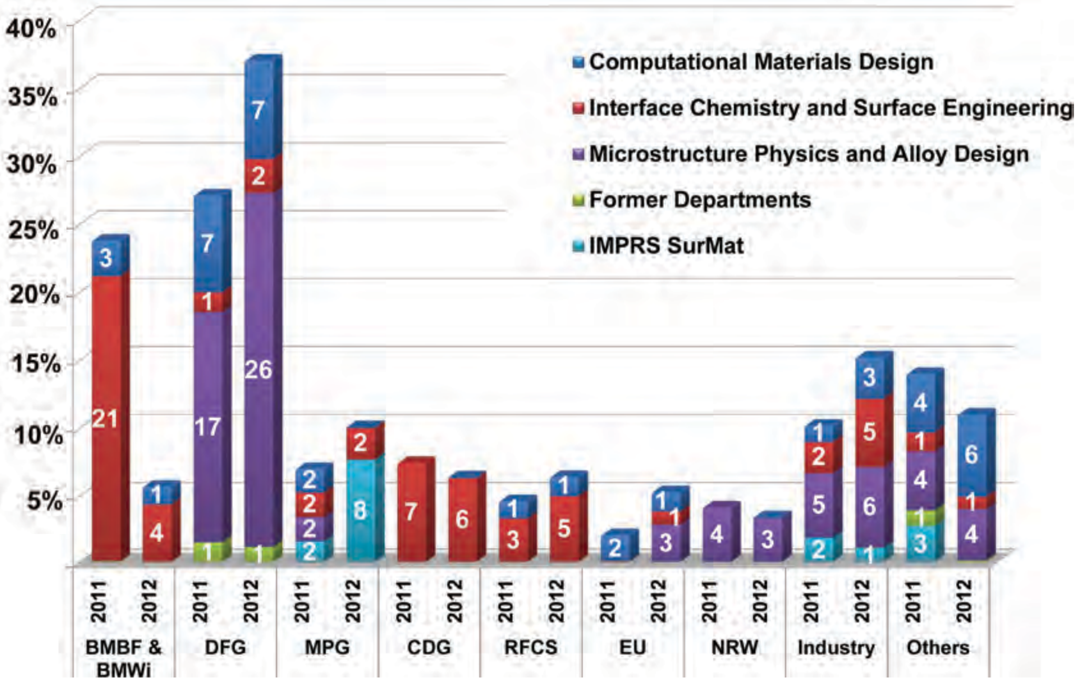
## Expenditure

(percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2012 data estimated)



## Third-Party Funds

(percentual contributions to total revenue including personnel, materials, investments; year 2012 data estimated)



numbers are rounded percentage values

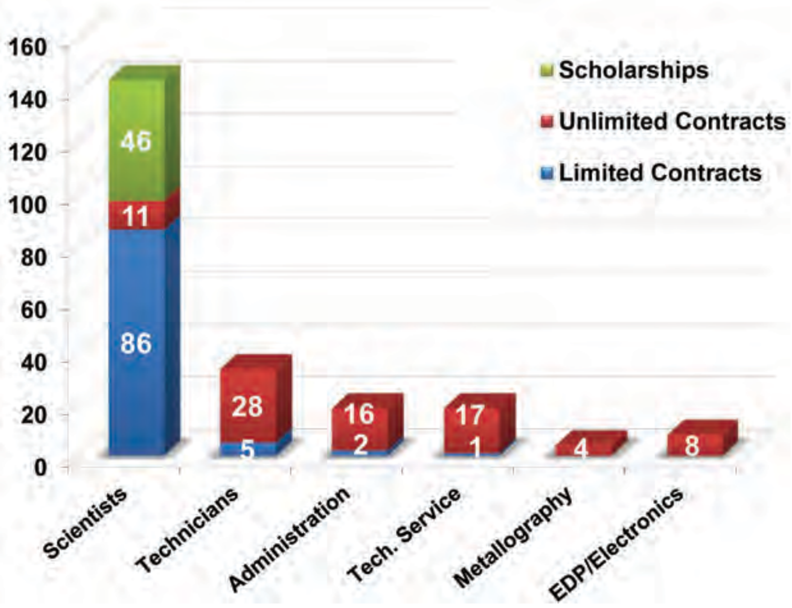
Former Departments:
Department of Materials Technology, Prof. G. Frommeyer, until Dec. 2008, and Department of Material Diagnostics and Steel Technology, Prof. A. Pyzalla, until Sep. 2008

BMBF: Federal Ministry of Science and Education
BMWi: Federal Ministry of Economics and Technology
DFG: German Science Foundation
MPG: Max Planck Society
CDG: Christian Doppler Society
RFCS: Research Fund for Coal and Steel
EU: European Union
NRW: State of North Rhine-Westphalia

# Personnel Structure

## Number of Occupied Scientific / Non-Scientific Positions

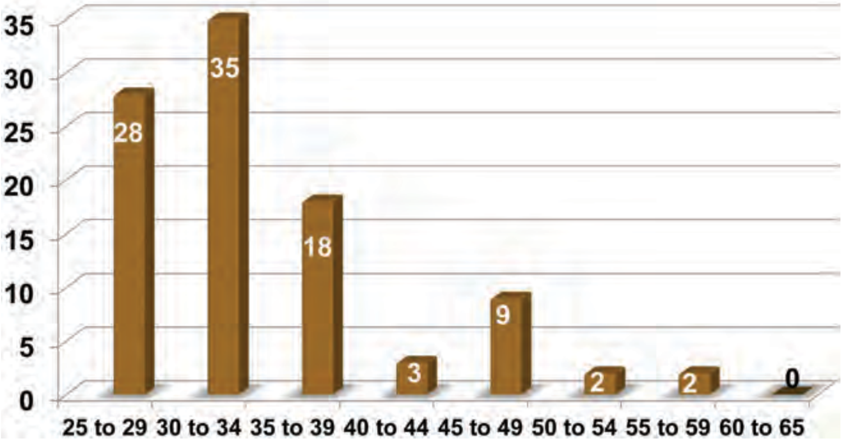
(Oct. 2012)



Additionally there were employed 15 interns and apprentices and 15 student research assistants.

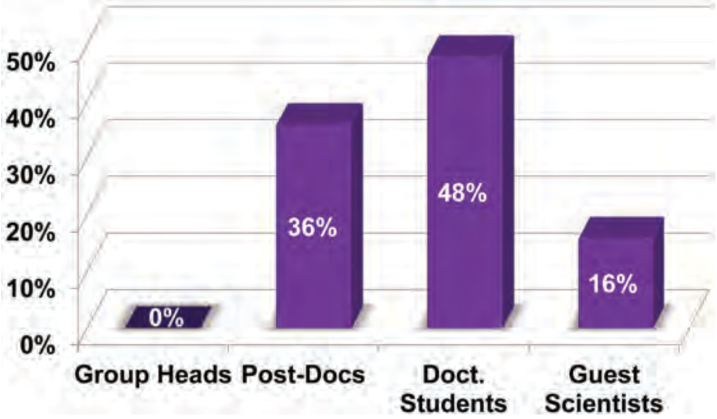
## Age Distribution of Scientists

(Oct. 2012)

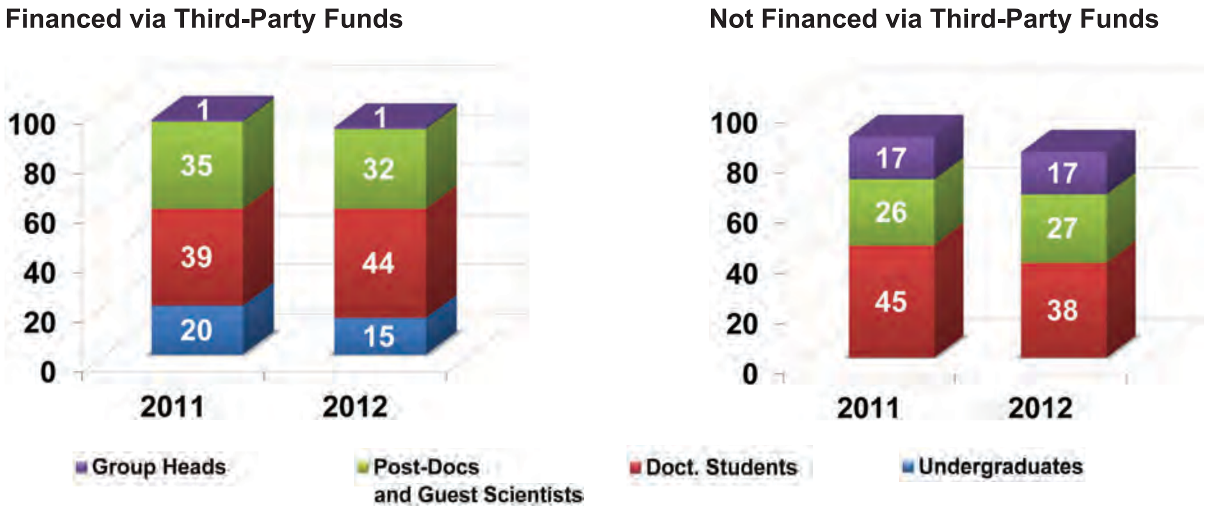


## Female Scientists

(Oct. 2012, percentual numbers)

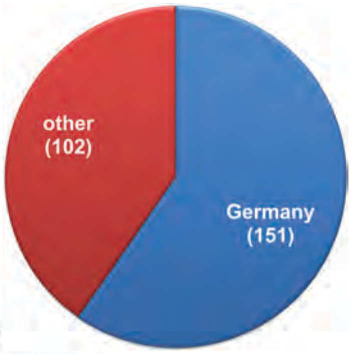


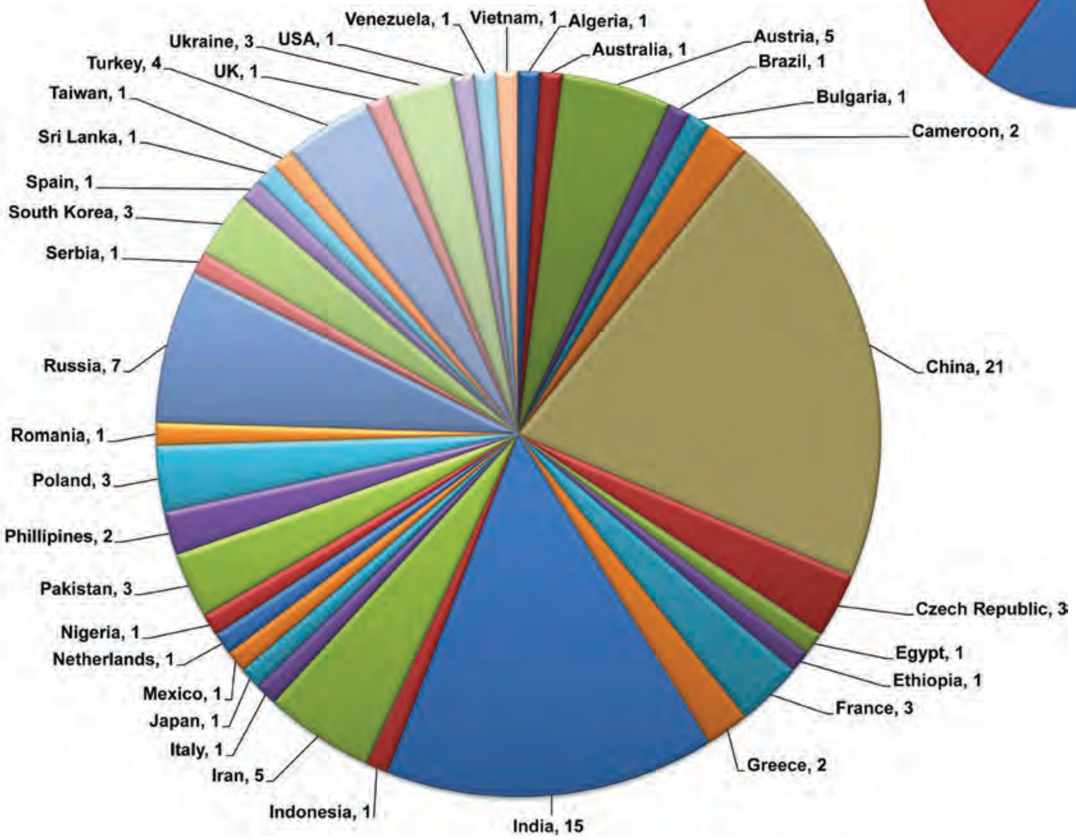
## Number of Junior Scientists (year 2012 data estimated)


**Financed via Third-Party Funds**

**Not Financed via Third-Party Funds**

## Employees and their Home Countries





# The Institute in Public

*Y. Ahmed Salem*

Public Relations

During the last two years the importance of public relations (PR) was enforced at the MPIE by the appointment of a press officer in April 2011. In the following, some major events and activities at the MPIE are described briefly.

## The MPIE in the Media

The number of published print and online articles about the MPIE could be more than tripled. This is not only due to the increased amount of published press releases but also to the creation of new mailing lists and a better internal communication which guarantees that important news are transported through the press officer to the public. In the following some important publications are named:

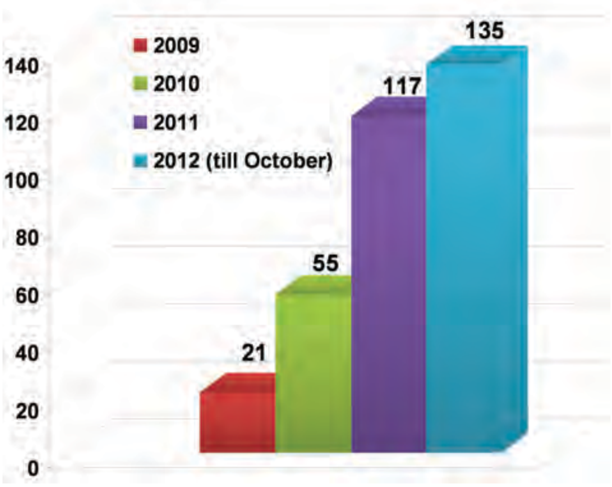


**Fig. 1:** *Amount of published print and online articles about the MPIE.*

- Rheinische Post: *“Humboldt-Stipendiaten zieht es nach Düsseldorf”*, 10 Aug. 2011
- Wirtschaftszeitung Aktiv: *“Stahl - was unsere Welt zusammenhält“*, 10 Sep. 2011
- Zeit: *“Auf höchstem Niveau“*, 13 Oct. 2011
- Westdeutsche Zeitung: *“Holländische Schüler im Max-Planck-Institut“*, 13 Oct. 2011
- Westdeutsche Zeitung: *“Eine Million Euro für das Max-Planck-Institut“*, 25 Oct. 2011
- Stahlmarkt: *“Düsseldorfer Stahlforscher überzeugten Worldsteel-Direktor“*, 01 Jan. 2011
- Stahl und Eisen: *“Computergestütztes Materialdesign optimiert Hüftimplantate“*, Volume 131, No. 11, 2011
- Umformtechnik: *“Metallforscher aus Düsseldorf und Japan kooperieren“*, Volume 4, 2011
- Max-Planck-Forschung: *“Die Rezeptur der Hummerschale“*, Volume 4, 2011
- Autocad-Magazin: *“Materialforschung: Superlegierungen für Triebwerke und die Energieversorgung von morgen“*, 07 Dec. 2011
- Maschinen Markt: *“Hochleistungsstähle erlauben Herstellung komplizierter Bauteile”*, 19 Dec. 2011
- Konstruktion und Entwicklung: *“Die Eigenschaftenvorhersager“*, Volume 01-02, 2012
- Innovationsreport: *“Intelligent corrosion protection“*, 03 May 2012
- Welt Kompakt: *“1,3 Millionen Euro für Forschung an Solarzellen“*, 01 June 2012
- Rheinische Post: *“Max-Planck-Preis für Fritz Körmann”*, 18 June 2012
- Süddeutsche Zeitung: *“Stahl aus dem Computer“*, 28 June 2012
- Stern.de: *“Stahl für übermorgen“*, 13 July 2012
- Stahl und Eisen: *“Stahl nach Maß - MPI-Wissenschaftler beim Ideenpark in Essen“*, Volume 132, No. 9, 2012

## Promotion of Young Scientists

As the promotion of young scientists in the field of material sciences, physics and chemistry gets more and more important, the PR established new cooperations with neighbouring schools. Lab tours are offered for the pupils, as well as the possibility to do an internship in one of the scientific groups or in the apprenticeship working stations. The institute was not only frequently visited by pupils but also by students, often from abroad. In 2012 students of chemistry, applied physics, metallurgy and material sciences from the Universities of Leiden and Delft (The Netherlands), from the Western Australian School of Mines (Australia) and from the University of Leoben (Austria) paid a visit to the institute. They were especially interested in experiencing how an international research institute works and in getting into contact with scientists in the field of modern material sciences.

Additionally, the MPIE took part at the “Science Days 2012” of the Theodor Fliedner Gymnasium on March 1rst and 2nd. During these days, one of the MPIE scientists, Dr. Sebastian Klemm, presented his work to pupils of different ages in the school. The MPIE also presented its work about TiNb- alloys for hip replacement at the “Highlights der Physik” in Rostock from September 26th to October 2nd. This event is promoted by the Federal Ministry of Education and Research and the German Society of Physics (Deutsche Physikalische Gesellschaft) and aims at explaining physics to a broad public.

**Fig. 2:** *Scientists of the MPIE and the RWTH Aachen explained how computer simulations work at the ThyssenKrupp Ideenpark 2012.*

On November 11th 2011 the institute opened its doors for pupils during the Max Planck Day. This day is announced by the Max Planck Society and is dedicated to pupils of different ages. Pupils have the chance to get in touch with the nature of science and experience science by themselves. In the second half of August 2012 the institute was also a partner of the ThyssenKrupp Ideenpark in Essen, a technical fair for young and old. There, the department of Prof. Jörg Neugebauer together with the RWTH Aachen presented the collaborative research centre 761 “Stahl *ab initio*” and showed how computer simulations help to develop new steels.

## VIP Visits

The institute had several VIP visits during the last two years. The North Rhine Westphalian state secretary Franz-Joseph Lersch-Mense visited the MPIE on June 15th 2011. He was fascinated by the work done at the institute and its unique structure as a public private partnership. Besides a lab tour where scientists of the MPIE explained their work, Lersch-Mense, Prof. Jörg Neugebauer, head of the department Computational Materials Design, Jürgen Kerkhoff, president of the Steel Institute VDEh and his vize-president Dr. Peter Dahlmann discussed the importance of Düsseldorf as a centre for research and talked about the diverse German research landscape.

Dr. Edwin Basson, CEO of the World Steel Organisation, paid a visit to the institute on September 20th 2011. Prof. Martin Stratmann, head of the department Interface Chemistry and Surface Engineering, explained how basic research in material sciences helps to develop new materials for the areas mobility, infrastructure and energy. Basson was impressed by the modern techniques used at the institute such as the three dimensional atom probe and the ultrahigh vacuum cluster.

On January 11th 2012, Thomas Jarzombek, member of the German Bundestag on behalf of the Christian Democratic Party (CDU), visited the MPIE on invitation of Prof. Stratmann. He was especially interested in the work of Dr. Karl Mayrhofer, head of the group Electrocatalysis. Mayrhofer got for his research project "ECCO$_2$ - combinatorial electrocatalytic CO$_2$ reduction" a funding of about one million euro from the Federal Ministry of Education and Research (BMBF). Jarzombek heard about this funding through a press release published by the MPIE.

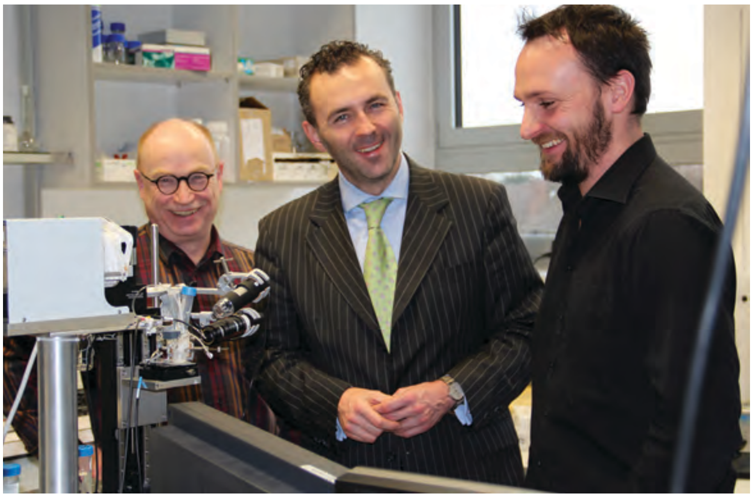
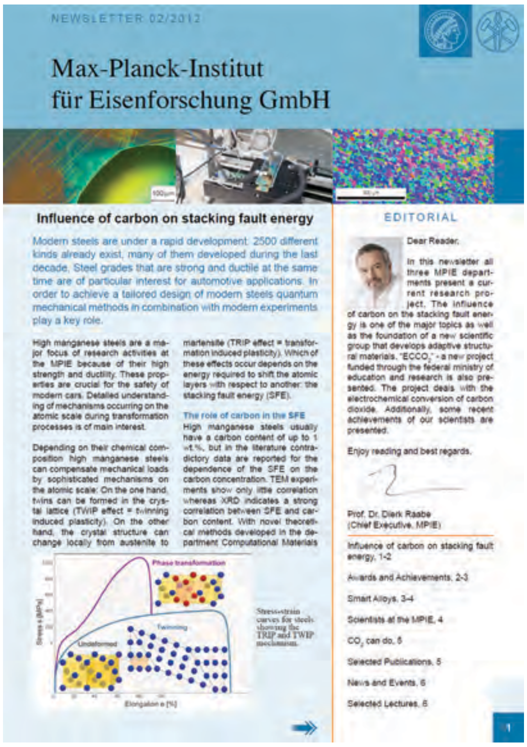


**Fig. 3:** *Dr. Karl Mayrhofer (right) and Prof. Martin Stratmann (left) explain to Thomas Jarzombek, member of the German Bundestag, how combinatorial electrocatalytic CO$_2$ reduction works.*

### Newly Launched Newsletter

Since the beginning of 2012 the PR publishes a newsletter which appears twice a year and provides information about recent developments at the institute, addressing main research achievements, technological breakthroughs and new instrumentation. The newsletter intends to build a bridge between basic science and application. Additionally, the team that stands behind the work is presented.



NEWSLETTER 02/2012

Max-Planck-Institut
für Eisenforschung GmbH

Influence of carbon on stacking fault energy

Modern steels are under a rapid development: 2500 different kinds already exist, many of them developed during the last decade. Steel grades that are strong and ductile at the same time are of particular interest for automotive applications. In order to achieve a tailored design of modern steels quantum mechanical methods in combination with modern experiments play a key role.

High manganese steels are a major focus of research activities at the MPIE because of their high strength and ductility. These properties are crucial for the safety of modern cars. Detailed understanding of mechanisms occurring on the atomic scale during transformation processes is of main interest.

Depending on their chemical composition high manganese steels can compensate mechanical loads by sophisticated mechanisms on the atomic scale: On the one hand, twins can be formed in the crystal lattice (TWIP effect = twinning induced plasticity). On the other hand, the crystal structure can change locally from austenite to martensite (TRIP effect = transformation induced plasticity). Which of these effects occur depends on the energy required to shift the atomic layers with respect to another: the stacking fault energy (SFE).

The role of carbon in the SFE

High manganese steels usually have a carbon content of up to 1 wt.%, but in the literature contradictory data are reported for the dependence of the SFE on the carbon concentration. TEM experiments show only little correlation whereas XRD indicates a strong correlation between SFE and carbon content. With novel theoretical methods developed in the department Computational Materials

Stress-strain curves for steels showing the TRIP and TWIP mechanisms.

EDITORIAL

Dear Reader,

In this newsletter all three MPIE departments present a current research project. The influence of carbon on the stacking fault energy is one of the major topics as well as the foundation of a new scientific group that develops adaptive structural materials. "ECCO$_2$" - a new project funded through the federal ministry of education and research is also presented. The project deals with the electrochemical conversion of carbon dioxide. Additionally, some recent achievements of our scientists are presented.

Enjoy reading and best regards,

Prof. Dr. Dierk Raabe
(Chief Executive, MPIE)

Influence of carbon on stacking fault energy, 1-2

Awards and Achievements, 2-3

Smart Alloys, 3-4

Scientists at the MPIE, 4

CO$_2$ can do, 5

Selected Publications, 5

News and Events, 6

Selected Lectures, 6

1

**Fig. 4:** *The newsletter of the MPIE appears twice a year and informs about recent research projects and the scientists behind the work.*

### Research Presented in Multimedial Gateways

The PR of the MPIE engages in the Max Planck Science Gallery and the Max Planck Science Tunnel. These multimedial gateways into the world of modern research were recently established by the Max Planck Society and present, under regularly changing topics, many research projects of the Max Planck institutes. While the Science Gallery is installed in Berlin, the Science Tunnel is a mobile exhibition that started in 2012 in Paderborn and will travel e.g. through Russia, China and Brazil. The MPIE is represented through several topics in these exhibitions. In the Science Gallery the topics multiscale simulations, corrosion, lightweight design and modern techniques of analysing materials are addressed. The last mentioned topic was also used for the Science Tunnel. There, a special focus lies on the three dimensional atom probe tomography and on up to date electron microscopy.

**Fig. 5:** *The ultrahigh vacuum cluster - a modern technique for analysing the surface of materials - is one of the topics presented at the Max Planck Science Gallery.*