Scientific Report
2009 / 2010

Max-Planck-Institut
für Eisenforschung GmbH

MAX-PLANCK-GESELLSCHAFT

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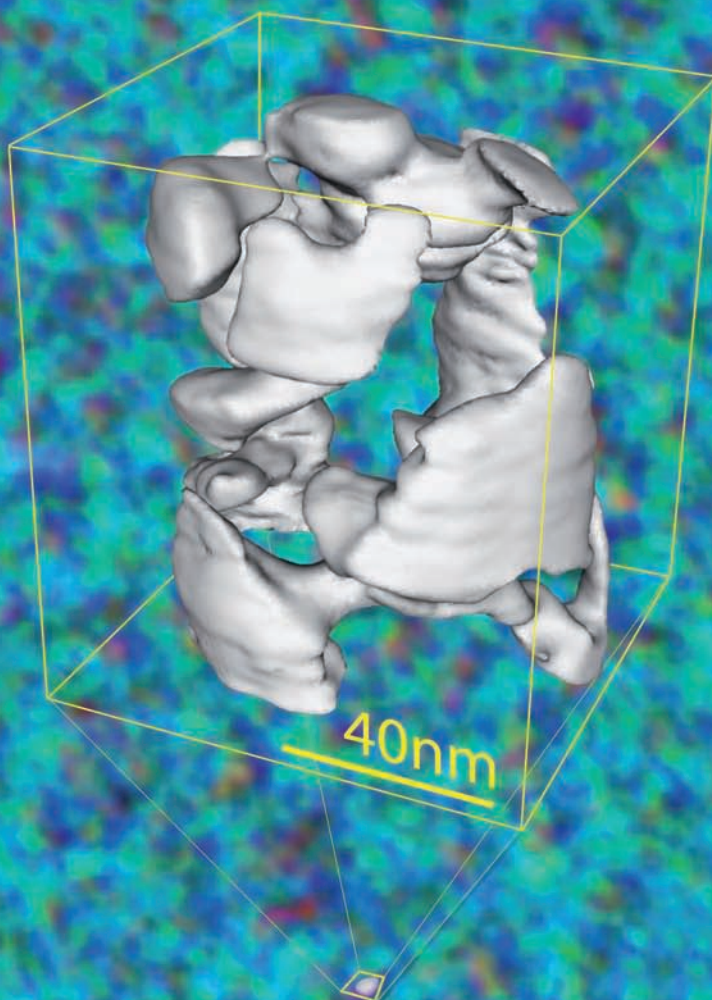
Max-Planck-Institut für Eisenforschung GmbH

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Front cover

Nanometer-scale analysis of a recrystallised, initially amorphous steel ($Fe_{50}Cr_{15}Mo_{14}C_{15}B_6$). The Scanning Auger Microprobe (SAM) image in the background exhibits the chemical composition of the recrystallised surface with a high resolution of 10 nm. Red shows Mo-rich, blue Cr-rich, and green Fe-rich regions. The chemical composition of the bulk of the material is evaluated by Atom Probe Tomography (APT) with a nearly atomic-scale precision. Shown in the figure is the Mo-rich part of the sample. The detailed analysis of the lateral variations in composition enables to understand macroscopic phenomena like corrosion behaviour (see p. 97).

PREFACE

This report is part of a series summarising the scientific activities and performance of the Max-Planck-Institut für Eisenforschung. In particular, this volume covers the years 2009 and 2010.

The MPI für Eisenforschung is worldwide one of the largest institutes devoted to fundamental research in steels and related structural materials, including their functional and surface properties, processing, and design. Projects are characterized by a highly interdisciplinary approach including close interfacing between experiment and theory.

The institute currently has three fully operative departments, namely, Computational Materials Design (J. Neugebauer), Interface Chemistry and Surface Engineering (M. Stratmann), and Microstructure Physics and Metal Forming (D. Raabe). The three groups reflect the broad scientific span that is covered in the institute ranging from quantum mechanics to electrochemistry and further to microstructure-property oriented process design of complex structural materials such as steels. 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 (forming, joining, coating), and materials properties (mechanical, stability, function).

The institute hosts about 260 people, the majority being scientists. To a large part the scientists working at the institute are supported by extramural sources. The 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 strategic and structural development of the institute during the past two years was strongly influenced by the retirement of G. Frommeyer and the appointment of A. Pyzalla as manager of the Berlin Helmholtz Centre for Materials and Energy at the end of the year 2008. These two changes in the institute's leadership were in part compensated by pursuing a set of interim projects on alloy design and joining of complex structural materials. Profound strengthening of the institute's scientific profile was achieved by the recruitment of R. Kirchheim (materials physics and atom scale characterization) as an external scientific member of the Max Planck Society and G. Eggeler (high temperature alloys and energy-related materials) as a fellow of the Max Planck Society. With both colleagues a number of fruitful joint projects were initiated (exploring the limits of strength, creep in superalloys, atomic scale analysis of interfaces in superalloys).

This report consists of the following parts:

- *Part I* deals with 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 three departments and Part III contains selected 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 Simulations of Materials*.

- *Part IV* summarises the statistically relevant information of the institute.

Dierk Raabe
Düsseldorf, November 2010

CONTENTS

IN COMMEMORATION OF
Prof. Dr.-Ing. Georg Frommeyer

Prof. Dr. Georg Frommeyer, former head of the Department of Materials Technology at the Max-Planck-Institut für Eisenforschung, Germany, unexpectedly passed away on February 7, 2010 at the age of 66.

Prof. Dr. Georg Frommeyer was born on December 24, 1943, in Georgsmarienhütte near Osnabrück, Germany. After finishing school he did an apprenticeship in mechanical engineering, and two years later he started studying mechanical engineering and materials technology at the University of Applied Sciences Osnabrück. From 1966 to 1968 he was head of the materials testing laboratory of the Klöckner AG steel plant in Georgsmarienhütte. In 1968 Georg Frommeyer began studying material science and metal physics at the technical universities in Aachen and Clausthal. After graduation (Diplom) he worked as a scientific assistant at the Institute for Material Science and Metal Physics at TU Clausthal. During this period he worked for a short time at the University of Liverpool. In 1973 Georg Frommeyer earned his doctoral degree (Dr.-Ing.) with the thesis "Mechanical and physical anomalies of highly deformed Ag-Cu compound alloys with extremely thin nano-structured fibres". Afterwards, as a junior scientist, he was project leader of the collaborative research centre "Solid state reactions in the bulk and at surfaces" of the Deutsche Forschungsgemeinschaft (DFG) at the universities Göttingen and Clausthal. Georg Frommeyer earned his habilitation in metal science and metal physics on the topic „Properties of highly deformed fibre- and layer-structured composites" in 1977. Between 1978 and 1980 he worked as a department head at the Fraunhofer Institute for Applied Materials Research in Bremen in the field of surface science and technology. In 1981 Georg Frommeyer was awarded a prestigious Heisenberg fellowship by the DFG which he spent with Prof. O.D. Sherby at the Department of Materials Science and Engineering at Stanford University, California. He came back to Germany in 1983

when he was appointed group leader and since 1990 head of the Department of Materials Technology at the Max-Planck-Institut für Eisenforschung in Düsseldorf. Here his main interests were the development and characterisation of steels and titanium alloys, the superplastic behaviour of materials, alloy design of novel light-weight high-temperature materials based on intermetallic phases, the analysis of atomic defects and ordering in intermetallic phases through atom probe field ion microscopy, rapid solidification of metals, and near net-shape casting. Since 1985, he was appointed as a professor at the Technical University Clausthal.

Particularly for the development of novel light-weight high-strength steels, Georg Frommeyer earned international recognition. His work is documented by more than 250 publications and 20 patents. In honour of his scientific achievements, Georg Frommeyer obtained numerous international awards, among them the Masing Gedächtnispreis of the Deutsche Gesellschaft für Metallkunde DGM (1974), the steel innovation award (1991 and 2000), the VDI award for innovative material applications 2008, the Vanadium Award of the Institute of Materials and Vanitec, London (1992) and the Materials Science Award 1996 of the Korean Institute of Metals and Materials, Seoul.

After reaching the age of 65 and instead of completely retiring from science, he continued his scientific activities and initiated the foundation "Mensch und Materie GmbH" where he was not only managing partner but also chairman of the scientific advisory board. He still had a lot of plans for future work.

On June 25, 2010, the Max-Planck-Institut für Eisenforschung organized a commemorative colloquium at the Steel Institute VDEh in honour of Georg Frommeyer, who has not only been an excellent and enthusiastic scientist but also an always optimistic and positive thinking, warm-hearted friend and mentor. We will always keep his honourable memory.

On behalf of the executive board and all employees at the Max-Planck-Institut für Eisenforschung

Dierk Raabe

Chairman of the Executive Board

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. 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 will be 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 Northrhine Westfalia, 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.

From 1971 until the present, 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.

Max-Planck-Institut für Eisenforschung GmbH
Management and Organization (2010)
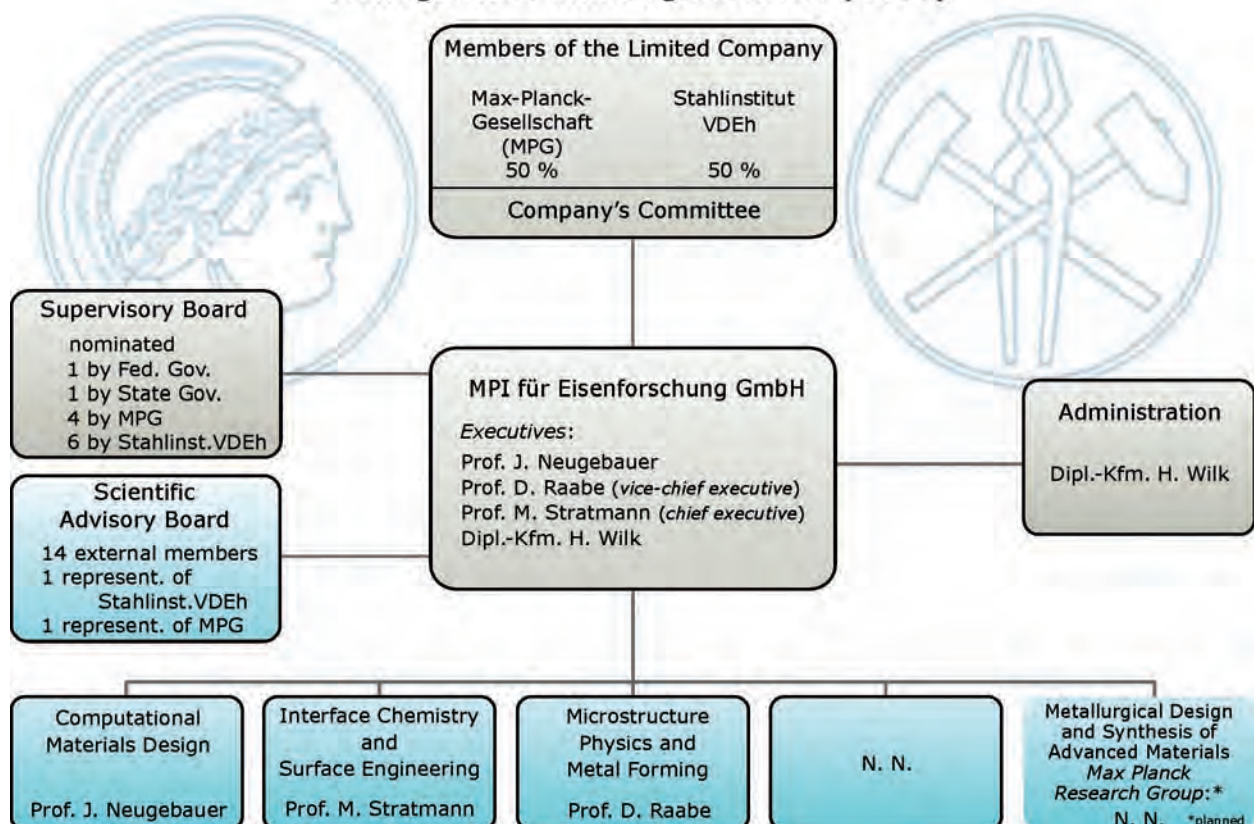
Scientific Organization

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 Metal Forming* (Prof. D. Raabe): mathematical modelling of microstructures and properties during processing and their experimental investigation using microscopy and diffraction methods

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

Scientific Scopes of the Departments

Computational Materials Design — Prof. J. Neugebauer	Interface Chemistry and Surface Engineering — Prof. M. Stratmann	Microstructure Physics and Metal Forming — Prof. D. Raabe
Ab Inito Calculation of Thermodynamic and Kinetic Data	Electrochemistry and Electrocatalysis in Energy Research and Corrosion	Mechanics of Materials
Theoretical Studies on Microstructure Properties and Dynamics	Adhesion and Coatings, Functional Surfaces and Interfaces	Microstructure and Texture
Alloy Design	Processes for the Controlled Production of Surfaces and Interfaces	Alloy Design and Thermomechanical Processing
		Biological Materials
		Atomic Scale Characterisation

- Stability of Surfaces and Interfaces

- Scale-Bridging Simulation of Materials

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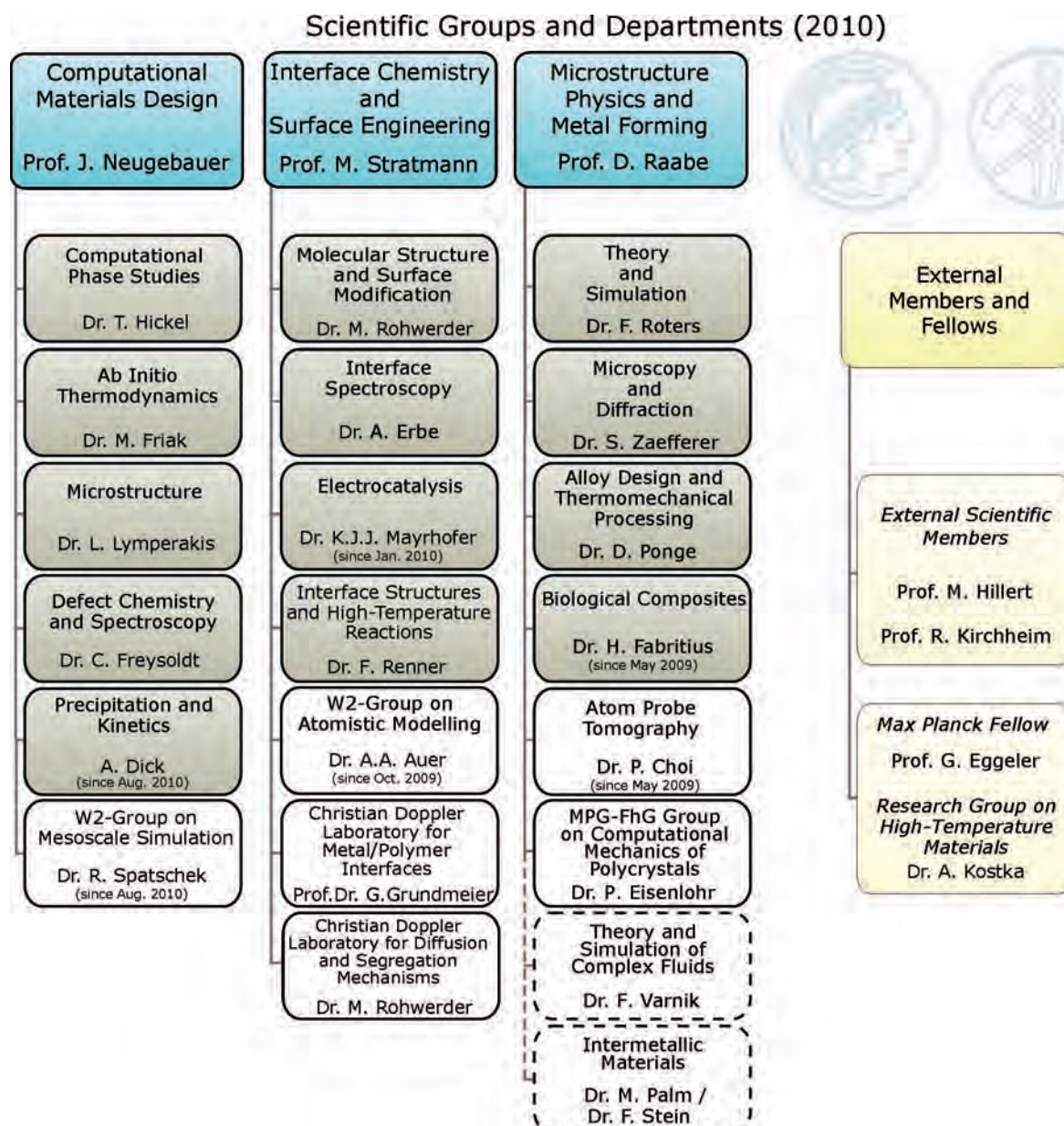
Service groups provide the scientific departments with valuable experimental expertise. These services include the production of materials, chemical analysis of metallic substrates, metallography, a mechanical workshop equipped for the handling of unusually hard and brittle materials, facilities to build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

Scientific Groups and Departments (2010)

Computational Materials Design Prof. J. Neugebauer	Interface Chemistry and Surface Engineering Prof. M. Stratmann	Microstructure Physics and Metal Forming Prof. D. Raabe	External Members and Fellows
Computational Phase Studies Dr. T. Hickel	Molecular Structure and Surface Modification Dr. M. Rohwerder	Theory and Simulation Dr. F. Roters	
Ab Initio Thermodynamics Dr. M. Friak	Interface Spectroscopy Dr. A. Erbe	Microscopy and Diffraction Dr. S. Zaefferer	*External Scientific Members* Prof. M. Hillert Prof. R. Kirchheim
Microstructure Dr. L. Lymperakis	Electrocatalysis Dr. K.J.J. Mayrhofer (since Jan. 2010)	Alloy Design and Thermomechanical Processing Dr. D. Ponge	
Defect Chemistry and Spectroscopy Dr. C. Freysoldt	Interface Structures and High-Temperature Reactions Dr. F. Renner	Biological Composites Dr. H. Fabritius (since May 2009)	
Precipitation and Kinetics A. Dick (since Aug. 2010)	W2-Group on Atomistic Modelling Dr. A.A. Auer (since Oct. 2009)	Atom Probe Tomography Dr. P. Choi (since May 2009)	*Max Planck Fellow* Prof. G. Eggeler *Research Group on High-Temperature Materials* Dr. A. Kostka
W2-Group on Mesoscale Simulation Dr. R. Spatschek (since Aug. 2010)	Christian Doppler Laboratory for Metal/Polymer Interfaces Prof.Dr. G.Grundmeier	MPG-FhG Group on Computational Mechanics of Polycrystals Dr. P. Eisenlohr	
	Christian Doppler Laboratory for Diffusion and Segregation Mechanisms Dr. M. Rohwerder	Theory and Simulation of Complex Fluids Dr. F. Varnik	
		Intermetallic Materials Dr. M. Palm / Dr. F. Stein	

T H E   I N S T I T U T E

Recent Developments

In the reporting period 2009/2010 the institute has been working with three departments: Computational Materials Design, Interface Chemistry and Surface Engineering, and Microstructure Physics and Metal Forming. In order to further develop the institute's expertise in complex materials we are currently identifying one or even two new directors for the institute. Areas of particular interest are advanced alloy design and synthesis as well as the structure and properties of novel complex materials.

The institute has recently significantly strengthened its scientific profile by recruiting internationally leading experts in the field of physical metallurgy. Prof. R. Kirchheim from the University of Göttingen accepted the offer to become an external scientific member of the Max Planck Society. He is well known for his achievements in fundamental aspects of materials science and in atom probe microscopy. Prof. G. Eggeler from the University of Bochum became a fellow of the Max Planck Society and established a research group on High Temperature Materials at our institute. The appointment of both colleagues allowed to initiate a number of highly active joint projects, which explore strength limits and creep in superalloys or interfaces in superalloys employing atomic scale analysis.

In the past two years a number of new scientific groups and topics have been established giving the institute a further bias towards covering an increasing variety of materials, systems, and properties of complex engineering materials. To accomplish this aim the institute was able to identify and hire top experts in internationally highly competitive areas and to establish new scientific working groups on atom probe tomography, precipitation and kinetics, mesoscale simulations, electrocatalysis, and atomistic modeling. The topics covered by these groups, their vision and the scientific background of the group leaders are presented in detail on pp. 15-20.

The combination of these new scientific activities with the already existing and well established expertise allowed the institute to even further strengthen the collaborations in house and to establish new external links and projects. For example, these developments further promoted our academic network with other Max Planck and Fraunhofer institutes (Max Planck Multiscale Modeling Initiative, Max Planck - Fraunhofer Initiative on Smart Surfaces, Max Planck - Fraunhofer Initiative on Polycrystal Mechanics) and with our neighbour universities RWTH Aachen (SFB 761) and Ruhr University Bochum (Max Planck graduate school SURMAT, Interdisciplinary Center of Advanced Materials Simulations (ICAMS), and Center for Electrochemical Sciences).

The increasing number of cooperations 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 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 cooperations are currently being developed in the fields of electro-mobility (soft magnetic steels for electrical engines and generators), battery research, and *ab initio* based methods for alloy design and damage tolerance predictions.

The new project directions will be highly 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 system, loading, and environmental conditions into advanced materials science and engineering projects. New areas of growth including strong interactions with new industry partners are envisaged in the fields of steels and related materials for automotive electro-mobility, energy storage, renewable energy conversion, and health.

New Research Groups

Atomistic Modelling

Group Head: A.A. Auer

Department of Interface Chemistry and Surface Engineering

The new atomistic modelling group in the department of Interface Chemistry and Surface Engineering has been set up in October 2009 by appointing Alexander A. Auer as new group leader (W2). A. Auer was formerly Juniorprofessor at the TU Chemnitz, where he is now appointed as Honorarprofessor. Besides the application of standard quantum chemical methods and algorithms to problems like the oxygen reduction reaction (see p. 57) or novel reactions in material science (see p. 61), work in the new group is focussed on the development and application of high-level first principles methods.

In the realm of their applicability, quantum chemical methods not only allow to interpret experimental data but also to predict molecular structures and properties. As a consequence, post-Hartree-Fock methods like Coupled Cluster (CC) or perturbation theory have achieved growing popularity during the last decades. The big challenge in the development of these approaches is to overcome the steep scaling of computational effort with system size that limits their applicability to smaller molecular systems.

The work in our group is focused on different aspects in the development of novel post-HF ab-initio approximations. This includes work on a refined local CC algorithm that incorporates an 'on the fly' screening of all wavefunction parameters based on sparsity estimates from perturbation theory. This way, low scaling of computational effort and smooth convergence of the energy as a function of the input thresholds can be achieved [1]. Another aspect is the application of decomposition techniques from applied mathematics (cooperation with the MPI-MIS Leipzig) to large dimensionality tensors as they appear in CC theory [2].

The high complexity of the working equations in post-HF methods renders method and code development very time demanding and error prone. A remedy for this problem is automatic code generation. One example for such a tool is the tensor contraction engine (TCE), which we have extended and applied to generate local CC methods and massively parallel implementations [3,4]. Current development is aimed at new embedding techniques based on local correlation methods that make highly accurate methods applicable to problems in surfaces science and electrochemistry.
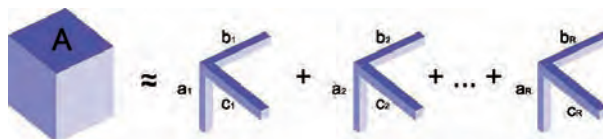
Tensor decomposition techniqes offer the possibility to overcome the curse of dimensionality by expressing multidimensional tensors as a series of lower dimensional objects.

The application of high-level ab-initio methods is focussed on the quantitative prediction of energetics and parameters in spectroscopy. Here, detailed studies have been carried out in order to evaluate the potential of state-of-the-art methods for the calculation of NMR parameters [5]. Furthermore, high level ab-initio methods have been applied in order to resolve questions from experimentalists in several recent studies [6,7].
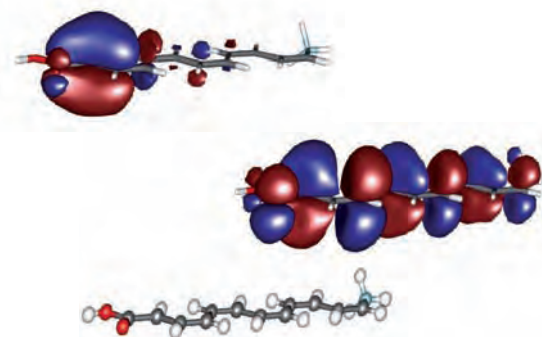
By using local orbitals (top) instead of delocalised canonical orbitals (middle) sparsity is introduced into the wavefunction parameters that can be exploited in local approximations.

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6. Bucher, G.; Grimme, S.; Huehnerbein, R. et al : Angew. Chem. Int. Ed. 48 (2009) 9971.

7. Auer, A.A.; Mansfeld, D.; Nolde, C. et al.: Organome-tallics 28 (2009) 5405.

Atom Probe Tomography

Group Head: P. Choi

Department of Microstructure Physics and Metal Forming

The research group for Atom Probe Tomography (APT) was established in May 2009. Its mission is to study changes in complex materials exposed to mechanical and thermal treatment and to understand structure-property relationships of advanced structural and functional materials at the nanoscale. A state-of-the art local electrode atom probe (Cameca LEAP 3000X HR), which yields three-dimensional elemental maps with sub-nanometer resolution, has been installed for this purpose.

Current research projects of the APT group deal with the investigation of precipitation, partitioning and segregation phenomena in high-strength alloys such as Mn-containing maraging TRIP steels and Ni-based superalloys as well as the mechanically and thermally induced changes in nanostructured materials such as cold-drawn perlitic steel wires and nitride multilayer hardcoatings. Functional steels under investigation are high strength softmagnetic FeSi alloys for electrical motors, which contain Cu nanoprecipitates. The changes in nanostructure upon thermo-mechanical treatment are related to the development of the mechanical properties of these systems. Besides structural materials, the APT group studies complex semiconductor devices for functional applications, namely thin-film solar cells and light-emitting diodes. With respect to these devices, the role of possibly existing dopants on the device performance is of primary interest. Local chemical fluctuations such as dopant clustering and segregation or partitioning to internal interfaces are investigated in systematic, site-specific APT analyses. Site-specific interface characterization (e.g. misorientation) can be conducted via Electron Backscatter Diffraction (EBSD) measurements in a dual-beam Focused-Ion-Beam (FIB) instrument that is used for APT sample preparation.

An important approach of our group towards a better understanding of the APT data is the correlation between experiment and theory. For instance, partitioning phenomena observed by APT in Mn-containing steels and Ni-based superalloys have been analyzed in terms of thermodynamic and kinetic calculations based on the Calphad method, using Thermo Calc and Dictra. Furthermore, comparative studies on nanoscale precipitation and Ostwald ripening phenomena based on first-principles calculations (Density Functional Theory) and statistical atomistic simulations (e.g. kinetic Monte Carlo method) are in progress.

One of the recent research highlights of the APT group is presented in the figures below. On the left side, the three-dimensional elemental map of a Ni-based superalloy (annealed at 700°C for 100 h), designed for the application in next-generation 700°C power plants, is shown. The sample contains several secondary $M_{23}C_6$ carbide particles near the grain boundaries, as confirmed by transmission electron microscopy. A plate-like $M_{23}C_6$ particle is resolved in the APT map. Furthermore, the ordered γ' phase has been formed at this carbide. Additions of boron that lead to a strong increase in the creep-rupture strength of this alloy are found to be segregated at the $M_{23}C_6/\gamma$ and $M_{23}C_6/\gamma'$ interfaces as shown in the composition profile. No boron segregation can be detected at the γ/γ' interface presumably due a small lattice mismatch between γ and γ'. Both boron segregation and the formation of γ' particles are believed to inhibit the growth of $M_{23}C_6$ particles and to be related to the superior creep properties of this alloy at 700°C.
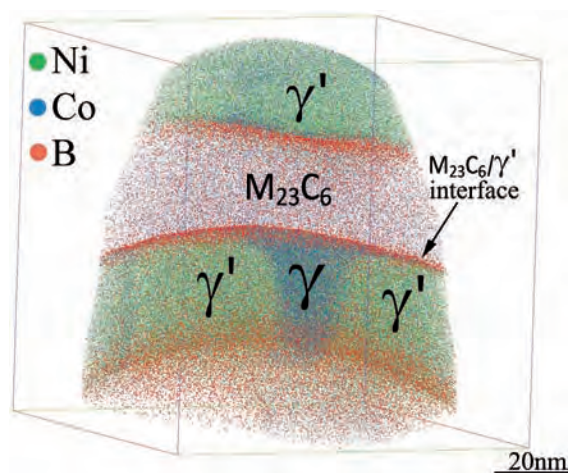
Three-dimensional elemental map of a Ni-based superalloy annealed at 700°C for 100 h.
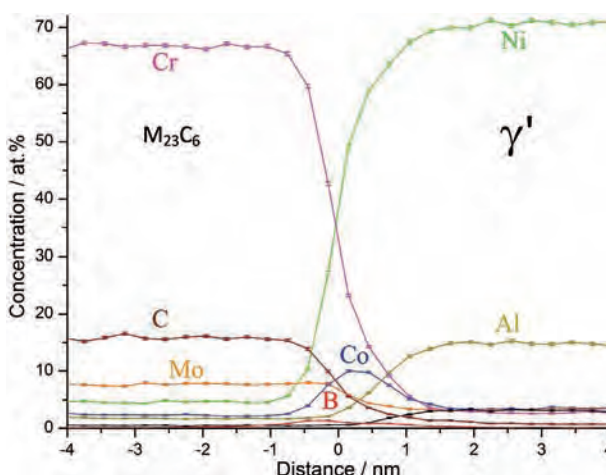
Composition profile across the $\gamma'/M_{23}C_6$ interface marked by the black arrow in the figure on the left side.

Precipitation and Kinetics

Group Head: A. Dick

Department of Computational Materials Design

The research objective of the group "Precipitation and Kinetics" initiated and headed by Dr. Dick in August 2010 is to provide accurate theoretical description on the time- and temperature-evolution of microstructure and phase transformations in multi-component multi-phase alloys based on first-principles calculations. The ultimate aim of the group activities is to develop methodology for calculating *ab initio* time-temperature-transformation (TTT) and time-temperature-precipitation (TTP) diagrams for industrially relevant materials, with the main focus on steels.

The evolution of microstructure upon thermo-mechanical treatment is on the most fundamental level related to single moves of individual atoms. Therefore, knowledge-based tailoring of material properties will in the future more and more relay on our capability to theoretically predict the underlying physical processes and events over a wide range of temperatures and stresses with high precision. *Ab initio* based techniques, being free of any adjustable parameters or experimental input data, in combination with simulation techniques to cover large length and time scales, promise an ideal starting point to achieve this goal.

The head of the group, Dr. Dick, is a leading expert in extending *ab initio* techniques to address complex materials and materials science problems. Making his PhD in 2008 on the development of *ab initio* simulation techniques to describe and understand magnetic probes with atomic resolution, he started a new research topic in the collaborative research center "Steel – *ab initio*". In this project, focused on description of extended defects in high-Mn steels at finite temperatures, he developed strategies to overcome the accuracy limits inherent to presently available conventional DFT methods and to achieve an improved accuracy needed for actual engineering applications (see p. 129).

The description of the microstructure evolution based on *ab initio* input is extremely challenging due to large gap both in length and time scales. The group will therefore analyze and employ combinations of molecular dynamics simulations for processes happening on the time-scale of lattice vibrations, and Metropolis and atomistic kinetic Monte Carlo schemes for time-scales characteristic for actual diffusion processes. Since realistic alloys are characterized by a huge configurational space, deriving all required parameters from explicit DFT calculations is not feasible. Therefore, the development and optimization of schemes which allow a mapping of DFT-derived parameters onto
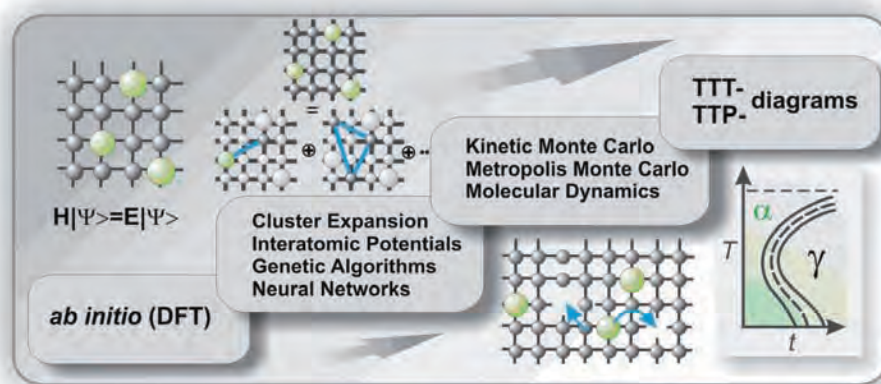
"Bottom-up" strategy to calculate time-temperature-transformation (TTT) and time-temperature-precipitation (TTP) diagrams from ab initio.

computationally efficient models such as, e.g., (spin) cluster expansion, genetic algorithms, interatomic potentials, will be one of the key tasks. A critical and not yet solved part is the inclusion of long-range strain effects (as induced, e.g., by lattice mismatch of the precipitates, extended defects or residual strain) into kinetic Monte Carlo simulations without compromising computational efficiency. The developed algorithms will be implemented employing the S/PHI/nX *ab initio* library package of the Computational Materials Design department.

First scientific projects in the group will be focused on investigating early stages of precipitation in maraging steels, studying the influence of the alloying elements on the thermodynamic properties of cementite precipitates in ferritic steels, and describing segregation and out-segregation of alloying elements at grain boundaries and stacking faults in high-Mn steels.

Biological Composites

Group Head: H. Fabritius

Department of Microstructure Physics and Metal Forming

From a materials science point of view, biological materials represent organic/inorganic composites with a hierarchical organization spanning over several levels from the nano- to the macro-scale. What makes these materials interesting study objects is that they have been optimized through evolution to perform vital functions within the specific eco-physiological constraints imposed on living organisms. These functions are very diverse and can be e.g. of mechanical, mobile, optical, or sensory nature. This diversity of physical properties is caused by structural and chemical alterations at different hierarchical levels.

The newly established research group Biological Composites is a multi-disciplinary group whose objective is to study the relationship between structure, composition and the resulting physical properties of biological materials in order to understand how nature designs structural materials with specific functions. The emphasis is on chitin-based materials, particularly the exoskeletons of Arthropoda and, to a minor extent, collagen-based materials such as bone. The Arthropod exoskeleton, the cuticle, consists of chitin and protein molecules that are organized in at least seven hierarchical levels (see figure below). It forms skeletal elements that all have in common the so-called twisted plywood structure, which is built by stacks of planar arrays of complex chitin-protein fibres. In some groups like the Crustacea, the organic material is combined with inorganic nano-particles. These particles are arranged according to the organisation of the chitin-protein fibres making the cuticle to a hierarchical composite material of high functional versatility. The aim of this research is to understand how and at which hierarchical level structural and chemical variations can lead to diversification of physical properties, with particular focus on the mechanical properties and behaviour of mineralized cuticles of different Crustacea and the optical properties of beetles (Insecta). Understanding and eventually applying the structure/property relations and the underlying design principles of cuticle in bio-mimetic approaches bears the potential for realization of a completely new generation of man-made structural materials.

This is achieved through a combination of experimental analysis and theoretical modelling. Experimental analysis is the core competence of the group and comprises characterization of microstructure, chemical composition and determination of the mechanical properties on all accessible length scales. Theoretical modelling is performed in a series of intra- and extramural collaborations and comprises *ab-initio* calculations for the molecular scale and hierarchical multi-scale modelling for the higher hierarchical levels of the materials.
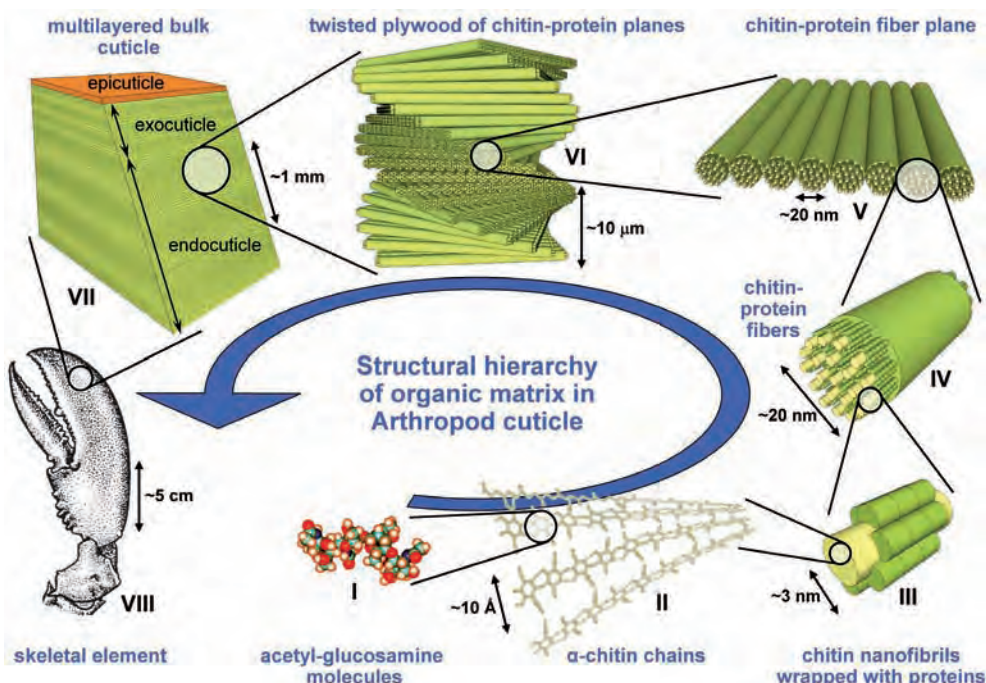
Hierarchical organization of chitin and proteins in Arthropod cuticle. Acetyl glucosamine molecules (*I*) form anti-parallel chains of α-chitin (*II*). Chitin chains wrapped with proteins form nanofibrils (*III*) which aggregate forming chitin protein fibres (*IV*) that are arranged parallel in horizontal planes (*V*). Stacked planes form the twisted plywood structure (*VI*) of the three-layered bulk cuticle (*VII*) which is used to build skeletal elements.

Electrocatalysis

Group Head: K.J.J. Mayrhofer

Department of Interface Chemistry and Surface Engineering

The electrocatalysis group was founded as part of the Department of Interface Chemistry and Surface Engineering in 2010. In general our research interests are electrochemical reactions at the solid-liquid interface, both without utilization of the released energy (corrosion) and with electrical energy conversion (batteries, fuel cells). The main focus of the group is placed on the concerted investigation of the activity, stability and selectivity of electrode materials for such heterogeneous reactions. This is achieved by a versatile combination of electrochemistry with complementary techniques for surface characterization and reaction product determination, as well as by the investigation and comparison of the behaviour of well-defined and real material surfaces.

The investigation of the properties of materials for electrocatalytic applications must be reliable, efficient, fast and inexpensive. The testing of catalysts in real systems or in conventional electrochemical setups, however, requires large amount of catalytic material and/or too much time for electrode preparation. Therefore high-throughput combinatorial screening tools play a major role in the installation of the modern electrochemical methodologies of the group. Moreover, the complementary techniques are incorporated effectively by utilizing sophisticated automatization and synchronization of the experimental setup, as well as advanced methods for data evaluation and processing. With this approach, a large number of samples can be systematically investigated in shorter time; while the reliability and reproducibility also increases. So for instance even the conventional Rotating Disc Electrode setup (RDE) is installed with automatic control of the experimental conditions such as the gas purging, in

ECat Team: K.J.J. Mayrhofer, I. Katsounaros, H. Venzlaff, N. Hodnik, J. Meier, S. Klemm, A. Karschin, A. Topalov, and A. Mingers (not on photo)

order to provide faster and more accurate results. Additionally, the excellent previous development of the Scanning Droplet Cell is further refined and combined with for example reaction product determination by Inductively Coupled Plasma Mass Spectrometer (ICP-MS, see p. 23). Synchronization of the methods and sophisticated data evaluation is indispensable for the high-throughput approach in this case. All of this should provide the basis for the thorough investigations of various material classes reaching from noble metals to steel samples, from a fundamental as well as applied point of view. Together with the departmental and institutional research groups and their competencies regarding surface characterization techniques and theoretical modeling, we thus hope to successfully address some of the key questions in interfacial electrochemistry.
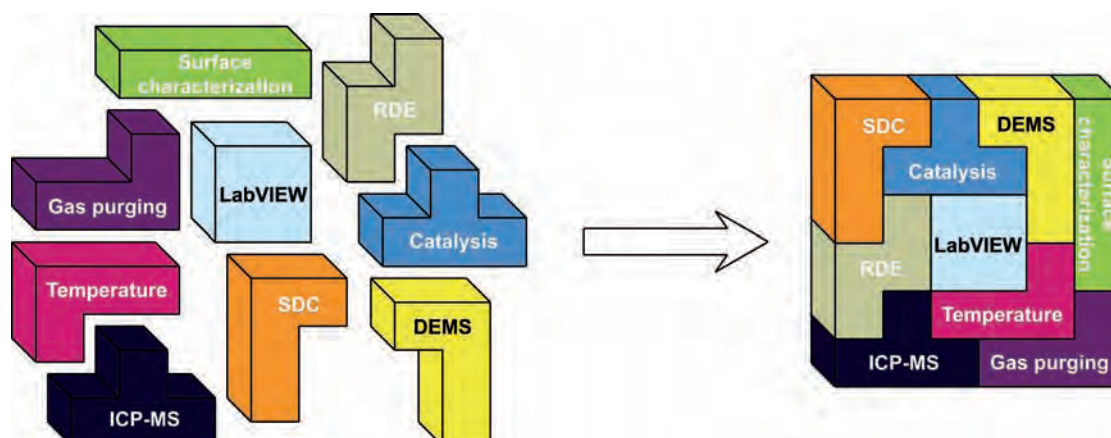

Automatization and synchronization of various techniques and experimental parameters as the foundation of the electrocatalysis group.

Mesoscale Simulation

Group Head: R. Spatschek

Department of Computational Materials Design

The behavior of materials is strongly influenced by the internal microstructure, which exists on a wide range of lengthscales, starting from individual defects and ranging up to complex grain structures. The formation of these inhomogeneities involves not only a large number of atoms but also takes place on timescales, which are much larger than typical atomistic timescales. The purpose of this newly established W2-group headed by Dr. R. Spatschek is therefore to extend the activities in the Department of Computational Materials Design to larger scales (both in space and time). Furthermore, the activities shall establish additional links to the Department of Microstructure Physics and Metal Forming concerning activities on macroscopic scales.
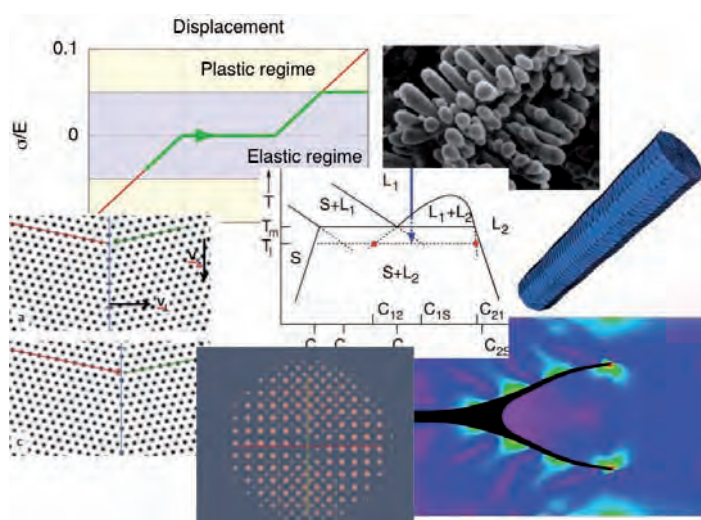
Sketch of activities in the mesoscale simulation group, which include plastic effects on the kinetics of phase transitions, monotectic reactions, morphological instabilities of nanowires, crack growth, dislocation and grain boundary dynamics.

R. Spatschek joined MPIE August 2010, and is currently installing a new research group. Before, he was group leader at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) at the Ruhr-University Bochum. The appointment shall further strengthen collaborations with this institute, and includes contributions to teaching activities in the new Master course "Materials Science and Simulation". R. Spatschek has a profound background in various aspects of mesoscale phenomena, including fracture mechanics, nonequilibrium interfacial pattern formation, solid-state transformations, elasticity, grain boundary premelting and coarsening phenomena. In the group various theoretical and numerical methods are available, including phase field models, Ginzburg-Landau descriptions, finite element approaches,

Green's function and boundary integral methods. Many of the underlying codes developed by him are designed to run on platforms ranging from single PCs up to massively parallel supercomputers. Furthermore, analytical methods are frequently used.

A selection of activitities, which have already been launched, is mentioned below:

The embrittlement of steels through hydrogen is of highest relevance for many technological applications. Together with the atomistic activities in the Department of Computational Materials Design, mesoscale descriptions based on amplitude equation approaches will be developed. This new description, which has been recently developed by the head of the group (R. Spatschek), goes beyond conventional phase field models by including an atomic resolution including lattice distortions and defect formation [1]. This allows to model the hydrogen distribution and dynamics of dislocations for investigation of the hydrogen enhanced local plasticity (HELP) mechanism on time scales relevant for this process, but not accessible with conventional atomistic (molecular dynamics) simulations. This activity is intended to be integrated into the SFB "Stahl ab initio".

Further activities are embedded into the DFG priority program 1296 "Heterogeneous nucleation and microstructure evolution", as a joint project with Prof. H. Müller-Krumbhaar, Research Center Jülich. The focus of the activities is related to elastic effects, as solid-state transformations in the presence of grain boundaries and interfaces, monotectic reactions, dissipative crack growth mechanisms and polycrystalline solidification.

Nanowires exhibit interesting physical properties and are promising e.g. for opto-electronic applications. Furthermore, on a continuum level, they are conceptually linked to whiskers, which cause difficulties in lead-free soldering. The understanding, controlled growth and suppression of these almost one-dimensional objects will be investigated. This project is performed in collaboration with Prof. A. Karma, Boston and ICAMS.

References

1. Spatschek, R.; Karma, A.: Phys. Rev. B **81**, 214201 (2010).

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New Scientific Laboratories and Facilities

## Atom Probe Tomography Laboratory

P. Choi

The new Max Planck Laboratory for Atom Probe Tomography (APT) was established in February 2010. APT is a characterization technique enabling spatially resolved chemical analyses of materials at sub-nanometer resolution (in-plane: $\Delta x = \Delta y \approx$ 0.2 nm; in-depth: $\Delta z \approx 0.1$ nm). The new 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

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 to a value of $\Delta m/m=1100$ (FWHM at $m/n = 27$). 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.
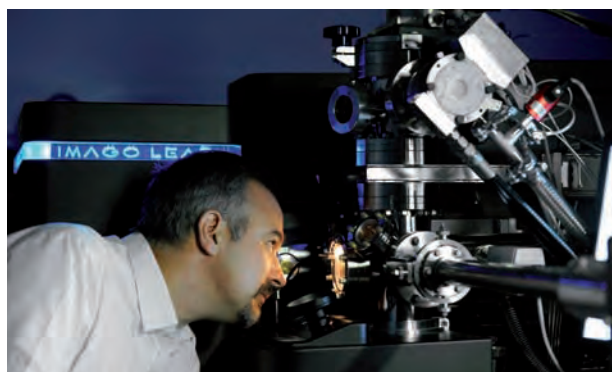
Local Electrode Atom Probe (Imago LEAP 3000X HR)

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 the specimen and the detector, the field of view can be
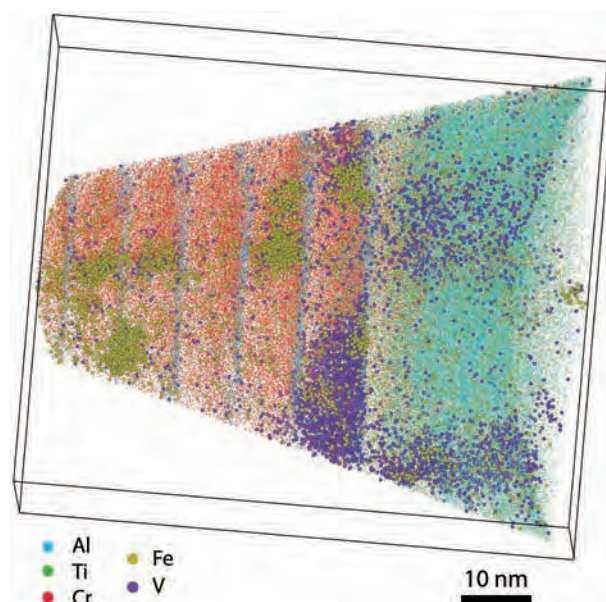
APT map of a TiAlN/CrN multilayer hardcoating annealed at 1000°C for 1h. Nitrogen atoms are not displayed for clarity. Fe and V impurities stemming from the steel substrate can be detected as well.

New High-Resolution Scanning Auger Microprobe

M. Rohwerder, S. Borodin, P. Keil

Scanning Auger microscopy is a powerful tool for investigating the chemical composition of surfaces, interfaces and thin films. A JEOL JAMP-9700F scanning Auger microprobe (SAM) was recently installed in the UHV laboratory of the GO department. It is equipped with a Schottky field emission gun, an electrostatic hemispherical analyzer with a multi-channel detector, an Ar-sputter gun, a neutralizer, a focused ion gun (FIB), a CCD camera to detect EBSD patterns, and an in-situ fracture stage.

Features of the JAMP-9700F include highest spatial resolution with probe diameters of down to 3 nm and 8 nm for SEI and Auger analysis, respectively. Additionally, a hemispherical analyzer type of electron spectrometer provides highest energy resolution allowing chemical state analysis of areas less than 10 nm. The installed scanning Auger microprobe system is ideally suited for studying chemical processes at the surface. The first projects with this new device include detailed investigations of the structure and corrosion of iron-based metallic glasses during crystallization and the selective dissolution of Cu_3Au on an almost atomistic level (see corresponding pages 97 and 62). Additionally, the installed system allows the investigation of grain boundaries und buried structures making use of the FIB (figure on the right) and/or the cleavage device (figure below).
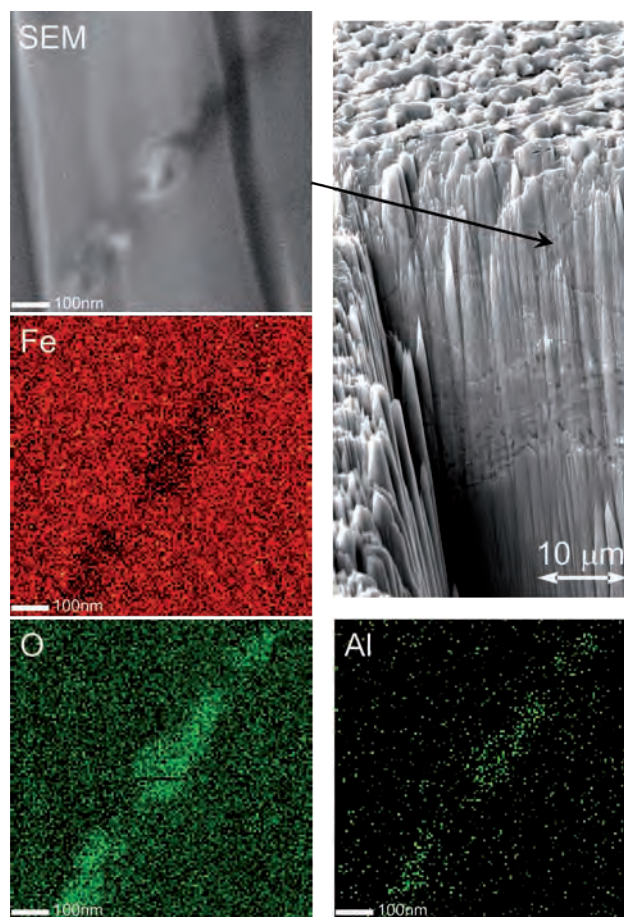
SAM map of a laid open grain boundary by means of FIB of Fe_3Al. The segregation of Al to the grain boundary and its selective oxidation due to the annealing in a forming gas atmosphere can be seen.
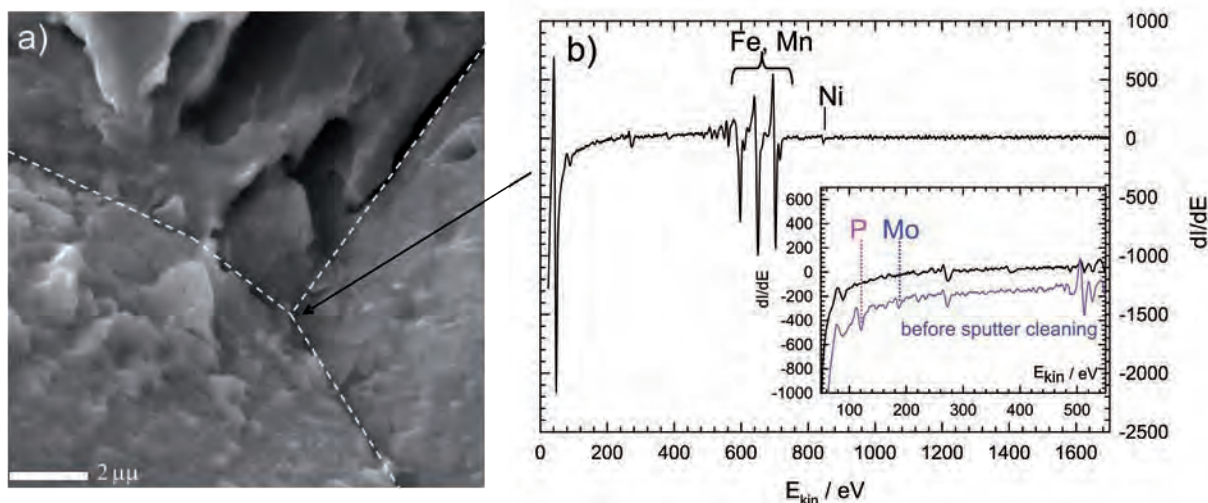
a) SEM photograph of Ni/Cr steel grade cleaved along grain boundaries. b) Auger spectra with 10 nm spatial resolution. The segregation of alloying elements like P or Mo can be demonstrated by sputter etching (black curve: after sputter etching of 5 nm, blue curve: before sputter etching).

Inductively-Coupled-Plasma Mass Spectrometry coupled with a Scanning Flow Cell

A. Mingers, A. Topalov, J. Meier, S. Klemm, I. Katsounaros, K.J.J. Mayrhofer

One of the main work horses in the newly founded electrocatalysis group in the Department of Interface Chemistry and Surface Engineering will be the combination of electrochemical experiments with an online multi-elemental analysis of the electrolyte. Therefore a commercially available Inductively-Coupled-Plasma mass spectrometer (ICP-MS) has been installed and is currently put into operation. The work principle of the ICP-MS is based on connecting inductively coupled plasma, as a method of generating isolated ions at 5.000 – 10.000 K, with a mass spectrometer that can subsequently separate and detect the ions depending on their mass to charge ratio. The ICP-MS is a fast multi-element analysis technique with low detection limits and high sensitivity for the determination of the sample composition. One spectrum over a range of 200 masses can be accomplished as fast as 0.05 sec; while with a recording speed of 0.1 s per mass a detection limit of even down to ppt can be obtained. Moreover it has a linear range of operation of up to 8 orders of magnitude, which enables a straightforward quantification of the amount of each component in the sample. In general and also in this specific setup the sample introduced into the plasma is in the liquid form, however also gaseous and solid samples could be analysed by this technique.

Due to these excellent properties of the ICP-MS it is a very suitable extension for simultaneous multi-element monitoring of dissolution processes during corrosion of bulk materials or degradation of noble metal catalysts for energy conversion. By coupling an electrochemical scanning flow cell (SFC; see highlight article on p. 121) to the ICP-MS the dissolved elements in the product stream are directly analyzed online. The integrated micro peristaltic pump of the ICP-MS is thereby utilized to suck the electrolyte through the SFC capillary over the working electrode surface and disperse it into the plasma. When the SFC is placed in close distance to the analyzer, the concentration of the elements in the electrolyte can be related almost in real time to the current-potential characteristics of the electrochemical experiment. Thus for instance the contribution of each individual element of an alloy material to the corrosion current density can be evaluated at different potentials, which can help to improve our understanding of passivation, surface segregation, and leaching effects. Of course the handling of the ICP-MS will be again automatized as far as possible and synchronized with the complete SFC setup, in order to incorporate it into the high-throughput material screening approach already from the beginning (see p. 19). Since the ICP-MS by itself and in particular in combination with the electrochemical measurements creates a flood of data, also the data evaluation will be designed to cope with that issue. This will significantly simplify the characterization of material libraries and the evaluation of corrosion properties in future.
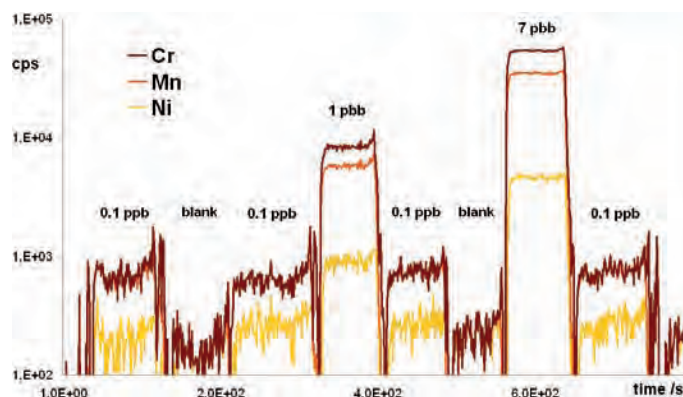
left: NexionTM 300 ICP-MS; right: First un-optimized calibration measurement for Cr, Ni and Mn; integration time 1 s; matrix 0.1 mol l⁻¹ NaCl; dispenser PFA 20 µl/s.

High-Performance Computer Cluster

A. Dick, W. Vogt, U. Wellms

The ab initio based simulation tools developed and applied in the Department of Computational Materials Design (CM department) and simulation activities in the other departments require a powerful high-performance computing (HPC) centre. To provide the necessary compute power, in the past years a state-of-the-art computer centre has been built based on concepts that combine flexible administration of heterogeneous compute architectures. It provides a flexible environment for the end-user, supporting simultaneously efficiency and flexibility with high security measures.

In February 2009 a new computer cluster had been installed in the CM HPC centre, increasing the number of CPU cores from 320 to 2216 and boosting the performance by a factor of roughly 10. The cluster has been optimized for time critical routines of the currently used simulation packages, which heavily rely on matrix-matrix operations (BLAS Level 3 calls) and fast inter-node communication via message passing interface (MPI). The estimated maximum theoretical performance of the cluster is 22.3 TFlop/s. Its actual performance has been measured with 19.34 TFlop/s (R_{max}), which is a site efficiency of 87%. Such a high efficiency could be accomplished by careful analysis and selection of the hardware components and by fine tuning critical kernel drivers. The cluster achieved rank 355 in the world-wide Top500 6/2009 list of high performance supercomputers and rank 24 in Germany. The current memory capacity of the CM Computer centre comprises approx. 5 TB RAM, 60 TB scratch space and 20 TB storage with backup.

In order to meet the increasing demands of compute power the Compute centre will be shortly upgraded: The number of CPU cores will be increased from 2216 CPU cores to approximately 7000 CPU cores. Since CPU performance and memory are tightly connected, the new cluster will be equipped with approx. 7 TB of RAM. In order to reduce the power consumption by the cluster, the cluster upgrade is performed using state-of-the-art energy-saving techniques, which allows constraining the required cooling capacity to less than 90 kW.

The huge amount of processes running simultaneously on a large-scale compute centre requires fast response times and high stability of all relevant network services. A traditional centralized administration approach utilized in the CM HPC so far will not be capable to achieve this on a setup of about 7000 CPU cores due to the scaling problems. Hence, the concepts behind the system are being updated to configure all services in a load-balancing and thus scalable and fully decentralized administration environment.

The storage services of the CM HPC centre will be upgraded accordingly in order to comply with the increased compute power. Therefore, a new 40 TB NetApp file server will be implemented. Scalable cluster storage is provided with a new 15 TB Panasas filer. It provides a parallel-access file system which will be connected to the cluster via the fast network interconnects (20 or 40 GBit/s via IP-over-IB).

Part of the computer cluster of the CM department and TOP500 certificate.

Large-Scaled and Networking Projects

The International Max Planck Research School for Surface and Interface Engineering in Advanced Materials:
Successful Evaluation and Extension for Further Six Years

R. Loschen, A. Erbe, E. Gattermann

Introduction. The International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS-SurMat) is an international graduate school which attracts students from all over the world. It is a joint project involving the Max Planck Institutes in Düsseldorf (MPIE) and Mülheim (MPI-KF) and the Ruhr University Bochum (RUB). In addition, three Chinese universities in Xiamen, Beijing and Shanghai are involved. The most important event in the IMPRS-SurMat of the past two years was the evaluation. For this reason, the SurMat programme was in a transition period over the last two years, resulting in fewer new fellowships.

Evaluation and extension. In April 2009 the SurMat was evaluated by four independent reviewers and a delegate from the Max Planck Society. They had to evaluate the scientific achievements as well as working conditions for participating students. The reviewers were "extremely impressed by the enthusiasm of the graduate students and by the scientific success of the school" and thus strongly recommended the extension for further six years of the programme. After the end of the first funding period in December 2009, 24 students had finished their PhD thesis, four of which with distinction. There are far more than 100 scientific articles published in peer-reviewed journals (see diagram on the right). Following the successful extension, two interview sessions were held in 2010, and a number of new students are in the process of joining the programme.

Organisation. Spokespersons of the IMPRS-SurMat remain Martin Stratmann (MPIE) and Gunther Eggeler (RUB). Together with three further members of the SurMat board they decide the direction of the programme. Organisational matters are handled by the coordination office, which is placed at the

MPIE in Düsseldorf. Rebekka Loschen remains the Administrative Director, while Andreas Erbe replaces Achim W. Hassel as Scientific Director, following A.W. Hassel's move to Johannes Kepler University Linz. Both directors are jointly responsible for the recruitment and the quality management of the school. Elke Gattermann joined the coordination office as assistant in 2009 and became a valuable member of the team assisting the board and the directors in all respects.

Students. The Research School aims at attracting talents from all over the world. The coordination office receives several hundreds of applications each year. Only a few percent of the applicants are admitted. Since the beginning in 2004 more than 60 students from 23 different countries joined the programme.
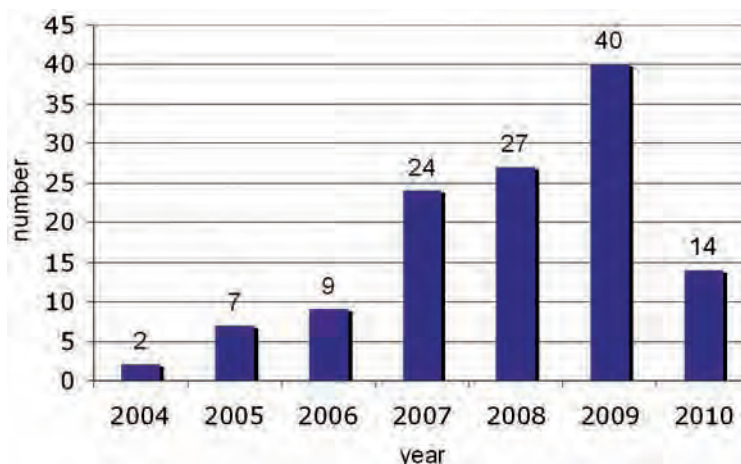
Publications by SurMat students since the start of the school in 2004.

More than 90% are from abroad (see figure on the next page).

Each student has two supervisors, usually from different fields. Thus good scientific communication and supervising is ensured, and the interdisciplinarity of the school is reflected.

Legend:
- Egypt
- Algeria
- Argentina
- Ethiopia
- Bangladesh
- China
- Germany
- Ecuador
- India
- Indonesia
- Iran
- Cameroon
- Colombia
- Lebanon
- Mexico
- Nigeria
- Poland
- Romania
- Taiwan
- Turkey
- Ukraine
- Belarus
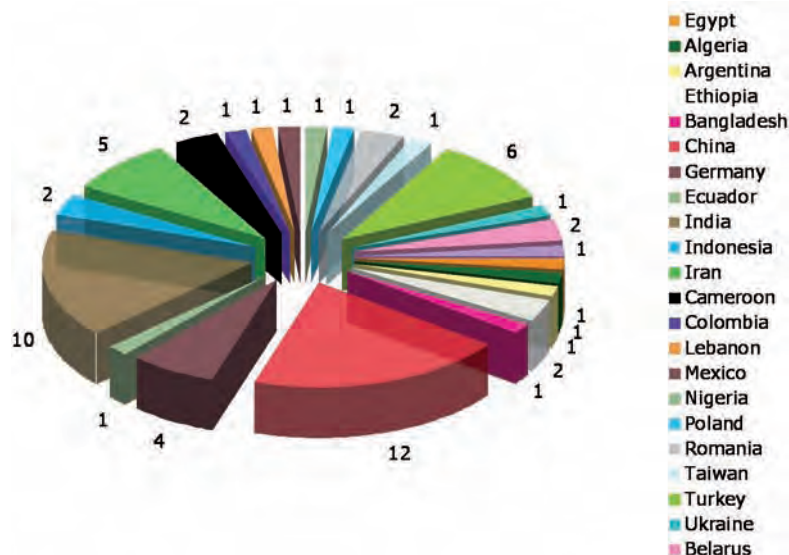
Origin of SurMat students by countries.

Some new features were introduced to improve the study experience. Annual reports will ensure a proper supervision. Additionally, the 2nd-year discussions allow for a well planned third year and thus shorten studying times.

Scientific Scope. The scientific expertise of the SurMat received a big boost by a number of partners from the field of theory and computer experiments. Starting from 2010, RUB's Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) has become a new valuable partner of the SurMat. The MPIE's Department of Computational Materials Design, which was not present at the time the SurMat was established, became a full partner. These new members complement the expertise from areas such as metallurgy, surface chemistry, corrosion and catalysis.

Outlook. Scientific collaborations with the Chinese partners will be rearranged in order to enhance the mutual student exchange.

A very important basis for improving cooperation is the new cooperation contract between the RUB, MPI-KF and the MPIE. Within this contract the position of junior scientists, who often are theses supervisors, are strengthened. Furthermore the involved departments agree that the logo of the Max Planck Society will be made visible on the PhD certificate after successful completion of the complete SurMat curriculum.

The changes made on the basis of the previous successful evaluation should be a sound basis for a fruitful second 6-year period of the SurMat.

Group photograph taken during the annual retreat in April 2010, Meschede.

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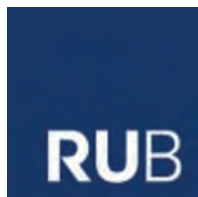
Center for Electrochemical Sciences

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

* Ruhr-Universität Bochum

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. The key missions of the center are the coordination of large-scale research projects of its members, establishing cooperations with external partners from industry as well as other research institutions, and the promotion of young researchers by funding their research activities and offering training courses in electrochemistry on different levels.

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 has already completed its first successful year, which was mostly coined by building a strong foundation for future research. Therefore a modern electrochemistry laboratory has been built up and equipped with various potentiostats including different electrochemical cells, an electrochemical quartz micro balance, impedance spectroscopy, scanning electron microscopy, atomic force microscopy, surface plasmon resonance, Raman spectroscopy and dynamic light scattering. This central laboratory is open to all members and associated members. In addition, three junior research groups working on "Molecular Nanostructures", "Semiconductor Electrochemistry", and "Adsorption and Electrocatalysis" have been established by three young experts in their fields, who have been selected from a large international list of applicants. Their research topics complement very well the work at the MPIE and RUB and therefore will enrich and broaden the existing expertise in electrochemistry. Various research projects have already been initiated by the CES members and they are as extensive as electrochemistry itself, however a vigorous synergy on certain hot topics like lithium ion batteries, the oxygen reduction reaction, biosensors, instrument development as well as theoretical electrochemistry is obvious.

The CES also aims at establishing a strong initiative of theory in Electrochemistry. Coordinated by A. Auer (MPIE) and R. Schmid (RUB) several projects are currently being initiated that include the applications of theoretical methods to problems from electrochemistry as well as the development of novel approaches for treating charged surfaces. In February and August 2010 two minisymposia on perspectives and challenges for electronic structure methods have been organised at the RUB and at the MPIE. More common initiatives and events are planned in future to further enhance the outcome of this promising networking project.

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

The idea and concept of ICAMS was developed several years ago by the MPIE and the Ruhr Area Initiative chaired at that time by the ThyssenKrupp Steel AG, in order to strengthen the long-standing competence in advanced materials in the Rhine-Ruhr area and to boost the already existing and foster new expertise in materials simulation. In March 2007 ICAMS was founded at the Ruhr-University Bochum (RUB). It is now supported by a consortium led by ThyssenKrupp Steel Europe AG, Salzgitter-Mannesmann Forschung GmbH, Robert Bosch GmbH, Bayer Materialscience AG and Bayer Technology Services GmbH, Benteler Stahl/Rohr AG together with the MPIE, the RWTH Aachen University and the state of North Rhine Westphalia.
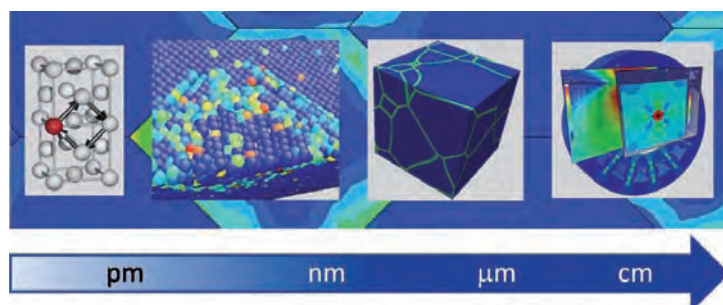
The objective of ICAMS and its partners like the MPIE is to develop the next generation of simulation tools for materials modeling and to transfer these simulation tools into industrial research and product development. As materials with specific properties become increasingly important for the development of new products, the goal of ICAMS is to guide the design of novel materials using computer simulations.

Since its foundation in 2007, ICAMS had focused on setting up infrastructure and on starting to fill the visions with life. The current structure of ICAMS with its three departments at the Ruhr-University Bochum and its three Advanced Study Groups (ASG) reflects the hierarchical multiscale structure of materials: Understanding bond formation, the electronic structure of a material and the time evolution of the re-arrangement of the atomic constituents are the main objectives of the Department Atomistic Modeling and Simulation (Prof. R. Drautz). The research of the Department Scale Bridging Thermodynamic and Kinetic Simulation (Prof. I. Steinbach) is focused on equilibrium and dynamic behavior of multiphase materials, linking the atomistic nature to the macroscopic scale. The Department Micromechanical and Macroscopic Modeling (Prof. Alexander Hartmaier) aims at deriving microstructure-property relationships to predict mechanical properties of materials.

The MPIE strongly supports these activities by running the ASG Modelling of ICAMS. This ASG, which is mainly situated in the Department of Computational Materials Design at the MPIE, is the organizational unit which combines the theoretical materials simulation activities in the institutes collaborating with ICAMS. It ensures a strong interaction and collaboration between the institutions and is actively involved in the research of ICAMS with individual projects, which aim at a better understanding of the properties of structural and functional materials at the atomistic scale by the means of *ab initio* methods.

The MPIE is also strongly involved in the teaching activities of ICAMS, being integrated in the faculties of Mechanical Engineering, Physics and Astronomy and the Masters Course Computational Engineering. The new international ICAMS Masters Course 'Materials Science and Simulation', which was setup and launched in fall 2010, covers modelling and simulation as well as experimental aspects of materials science. Members of the MPIE (Prof. Neugebauer, Dr. Hickel, Dr. Spatschek) are in charge for several modules belonging to the course.

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

T. Hickel, S. Zaefferer, F. Roters, D. Raabe, J. Neugebauer

In 2007 the Max-Planck-Institute in Düsseldorf (MPIE) and RWTH Aachen University jointly initiated a new 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), Fig. 1.

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. To achieve this goal 16 projects, organized in three research fields (Theory, Processing, Characterization), have been established. Scientists from the departments of Prof. Raabe and Prof. Neugebauer at the MPIE are currently responsible for four of these projects

The current phase of the project concentrates on the ternary Fe-Mn-C system, forming the basis of high manganese steels. Such alloys are prominent examples of next-generation high-strength steels, which exploit the TRIP and the TWIP effects for excellent forming and strain hardening characteristics (TRIP: transformation-induced plasticity; TWIP: twinning-induced plasticity). However, a better understanding of the fundamentals of thermodynamic, kinetic, and mechanical mechanisms is urgently needed. Further, this class of structural materials is well suited for this project as its thermodynamics and mechanical properties are sensitively influenced by the chemical composition. The obtained results reveal that these chemical as well as thermodynamic dependencies can efficiently be predicted and analyzed by *ab initio* studies. Accordingly, main thermodynamic properties such as the structure, stacking fault energies, and elastic properties have already been provided by the *ab initio* projects and are directly used in phenomenological plasticity models (see p. 129) and optimized thermodynamic data bases (see p. 131). In addition, experimental validation (see p. 107) and process technology developments are crucial for exploiting the extraordinary potential in terms of strength and ductility of high manganese steels.

Inspired by these successful results, SFB 761 will continue in the manufacturing and characterization of Fe-Mn-C-steels of different compositions, the use of *ab initio* methods for the prediction of key thermodynamic parameters (relevant, e.g., for TWIP, TRIP, shear band 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.

Scientists collaborating in SFB 761.

**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 (IAP) 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. This requires that a suitable trigger signal can travel through the coating or along the interface and activate a sufficient number of the stored capsules. Furthermore, similar to the electrochemical working mechanism of chromate, the process needs to be site selective, i.e. focused on the defect itself, otherwise there would be no chance to repair larger defect sites. The realization of this ambitious project will involve cutting edge experiments on the fundamentally underlying mechanisms such as how to optimize the directed transport of the active agents and the site selectivity of the repair action.
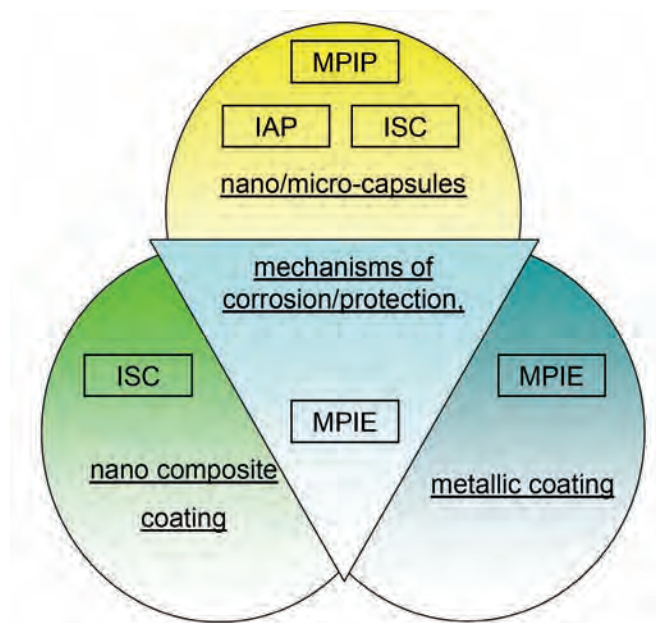
Cooperation partners and their main working fields within the ASKORR research project.

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

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

The general background for these activities is the world-wide need for alternative mobility schemes. On energy balance (well-to-wheel), electric drives are already more efficient compared with the internal combustion engine under today's power station mix and can thus contribute to a reduction in CO_2 emissions. The electrification of drives is crucial to the future of mobility. There is, however, still tremendous need for research, improvement and networking at many points in the supply chain. Greater efforts must be made in the key technology of storage batteries.

The German Federal Government's 2009 Economic Stimulus Package II includes measures to foster electrochemistry with an electromobility focus. The Center for Electrochemical Studies (CES), with its partners of the Max-Planck-Institut für Eisenforschung (MPIE) and the Ruhr-Universität Bochum (RUB), contribute in this framework to activities (Fig.1) within the "Northern Alliance for Competence" (Kompetenzverbund Nord, KVN), which is a project in line with the Federal Government's National Electromobility Development Plan[1]. Project leader is the Forschungszentrum Jülich (FZJ) and further partners are the universities of Aachen (RWTH), Münster (WWUM), and Hannover (LUH). Among the goals are an establishment of applied research priorities in electrochemistry at universities and non-academic research institutions, and the development of joint curricula for promotion of junior scientists.

New concepts are needed to meet the requirements of a real fleet of vehicles in terms of electrochemical functional parameters, safety and economy.

The figure shows the main fields of activities of the project on the basis of the value-added chain for electromobility. The MPIE is contributing studies on model interfaces and focuses thus on fundamental questions. The main aspect is the preparation of model interfaces and their characterisation using
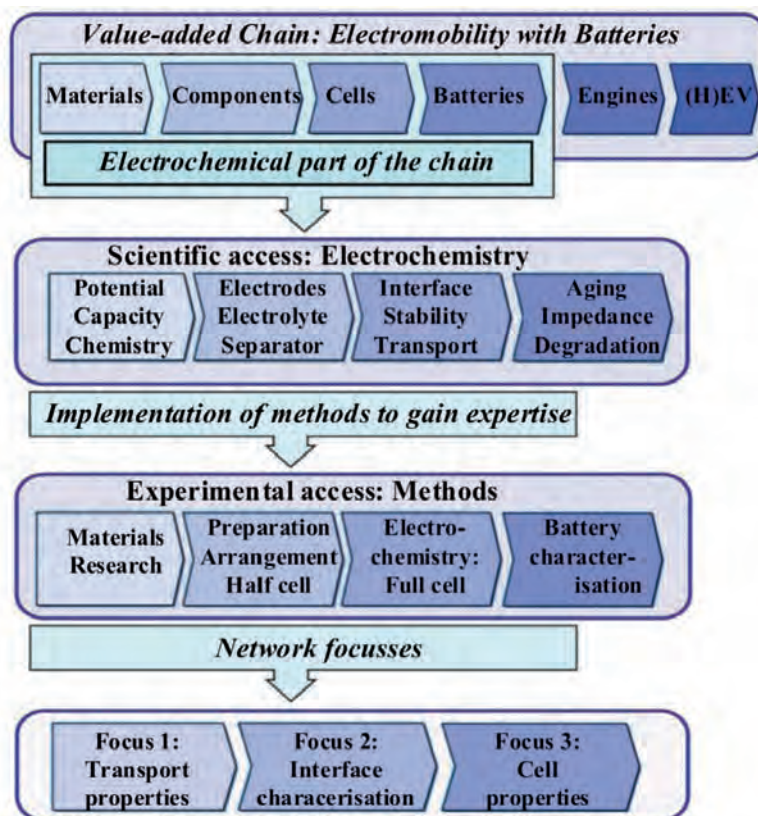
Value-added chain and project outline of the Northern Alliance for Competence (Kompetenzverbund Nord, KVN).

modern surface analytical equipment, such as atom probe tomography (APT), scanning Auger microscopy (SAM), and scanning Kelvin probes (SKP). Furthermore in-situ surface X-ray diffraction employing synchrotron light facilities will be used.

Simple model interfaces are single crystalline (like thin film systems), polycrystalline or amorphous substrates in contact with Li-containing ionic liquids and polymers. Within the project a new PLD chamber will be installed and used for the creation of model interfaces. The focus is set on a basic geometrical and chemical characterisation and the description of surface reactions and transport phenomena which occur on these model systems.

[1] http://www.bmvbs.de/SharedDocs/DE/Anlage/VerkehrUndMobilitaet/national-electromobility-development-plan.html

Aachen Institute for Advanced Study in Computational Engineering Science – AICES
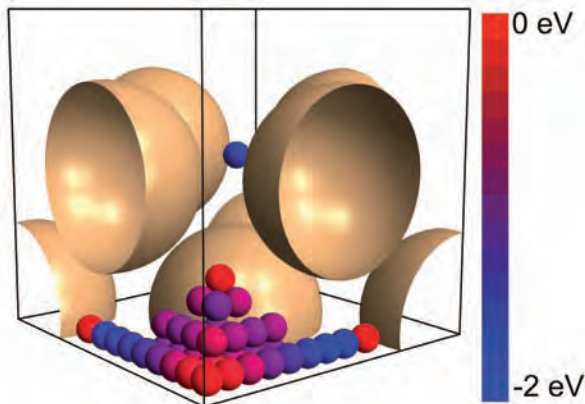
P. Eisenlohr, M. Friák, D. Raabe, J. Neugebauer

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. 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 http://www.aices.rwth-aachen.de).

The AICES program provides a multi-disciplinary training at the interface of classical engineering, materials science, applied mathematics, and computer science. The focal issues are method-oriented challenges within the simulation-based

Visualization of ab initio calculated total energies of C-containing Al matrix for different C positions with respect to a vacancy in Al. The larger spheres indicate Al atoms, smaller ones schematically represent a set of possible C positions with a color-coded total energy of the system (relative to the energy of the state with the C atom located in the centre of the vacancy).
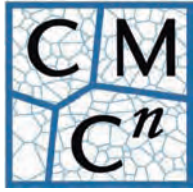
engineering science, as e.g. multi-scale problems bridging the gap between the atomistic and macroscopic properties and phenomena. The AICES Graduate School complements and extends existing research activities at both RWTH Aachen and MPIE. Dr. Philip Eisenlohr (department of Prof. D. Raabe) and Dr. Martin Friák (department of Prof. J. Neugebauer) became junior research group leaders associated with the AICES program during 2007.

Dr. Eisenlohr's research activities in connection with AICES deal mostly with aspects of interfaces in crystal plasticity, specifically the incorporation of slip resistance exerted by high-angle grain boundaries into crystal plasticity finite element (CPFEM) simulations and the identification of grain boundaries and associated mechanisms that are susceptible to nucleate damage (cracks or voids) upon localized plastic deformation.

Since early 2010, Dr. Friák and Dr. Hickel co-supervise the master thesis of one AICES-student, B. Sc. Nima Hamidi Siboni. The thesis entitled "Effect of interstitials on vacancy formation and mobility in metals" is focused on analyzing the impact that interstitial atoms (particularly industry-relevant elements such as hydrogen, boron, nitrogen or carbon) have on the concentration of vacancies (see figure) and, consequently, mechanical properties of metals. Due to the fact that an experimental study of the influence of impurities on the vacancy concentration is rather difficult and quite demanding, the method of choice for this investigation is a combination of theoretical parameter-free calculations based on fundamental quantum mechanics with statistical thermodynamics.

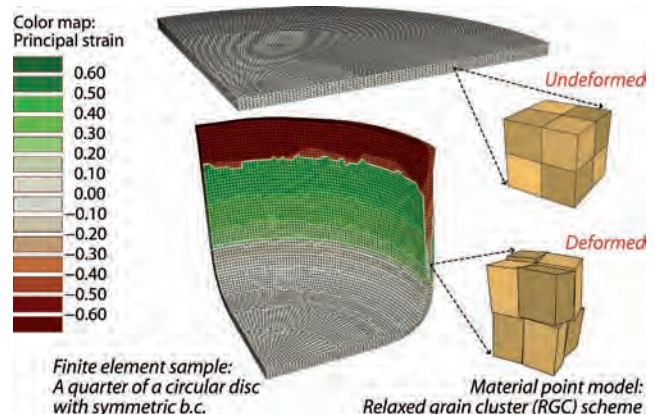# Computational Mechanics of Polycrystals – CMCⁿ

P. Eisenlohr, D.Tjahjanto, F. Roters, D. Raabe

Metallic materials of technical relevance are mostly polycrystalline and contain a large number of individual crystallites. During the manufacturing process the orientations of those constituting single crystals are altered and a non-random distribution typically evolves. Due to the anisotropic mechanical properties exhibited by single crystals, the polycrystalline aggregates also respond anisotropically to mechanical loading. Predicting the combined response of aggregated grains, which as a rule will experience non-uniform boundary conditions, is a challenge. However, research in this area has seen substantial progress in the last decade, such that combining modern continuum mechanical concepts with associated numerical solution strategies now opens the possibility to transfer fundamental metallurgical insights to industrially relevant problems in, for instance, the forming of multiphase sheet steel.

In this spirit, the Max-Planck-Gesellschaft and the Fraunhofer Gesellschaft in 2006 established their first-ever joint research initiative dealing with the topic "Computational Mechanics of Polycrystals – CMCⁿ" and having two strategic aims of accelerating knowledge transfer from fundamental sciences to applications and in parallel to build a long-term alliance between the Max Planck Institut für Eisenforschung (MPIE, Düsseldorf) and the Fraunhofer Institut für Werkstoffmechanik (IWM, Freiburg). The initial start-up phase of six years is supposed to fade into two tightly connected self-supporting working groups, one at each institute. Hence, acquisition of third party funds is integral to the initiative and currently well ahead of the anticipated amount of external funding. During 2009/10, the MPIE secured a new three-year PhD research project with the DFG, so that currently four full-time researchers are associated with the CMCⁿ initiative at the MPIE and six at the IWM.

The scientific goals of this initiative are set along two parallel lines: (i) a deeper metallurgical understanding of mechanical twinning, deformation induced phase transitions and multi-phase microstructures, and (ii) the optimization and acceleration of existing simulation methods both in Taylor-based and self-consistent texture modeling as well as in finite element method (FEM) based homogenization schemes. The four project leaders involved are focusing on the physical mechanisms of crystal plasticity (P. Eisenlohr), aspects of homogenization and numerical coarse-graining (D. Tjahjanto), efficient models of texture evolution (A. Prakash), and industrial demonstration and applicability (D. Helm) all of which have substantial mutual overlap.

Color map: Principal strain

| 0.60 |
| 0.50 |
| 0.40 |
| 0.30 |
| 0.20 |
| 0.10 |
| 0.00 |
| −0.10 |
| −0.20 |
| −0.30 |
| −0.40 |
| −0.50 |
| −0.60 |

Undeformed

Deformed

Finite element sample: A quarter of a circular disc with symmetric b.c.

Material point model: Relaxed grain cluster (RGC) scheme

An important achievement during the last two years was the implementation of a flexible material point model as a user subroutine. With this, arbitrary combinations of material constitutive laws and spatial detail from resolving individual grains up to a homogenized scale are possible within a single geometrical setup. This user subroutine is now used at both institutes and in different commercial FEM solvers. Another highlight was the application of a newly developed homogenization scheme based on a grain cluster model, which shares key features with the discontinuous Galerkin method, to cup drawing of ferritic–martensitic steel (see Figure) featuring computation times of less than an order of magnitude higher than standard iso-strain homogenization but with much improved predictability.

Current work in progress comprises on the side of improved physical understanding the development of a constitutive law that explicitly treats the dislocation advection, which is relevant in grain-scale plasticity and important to address questions of plastic accommodation in deformation-induced phase transformations / mechanical twinning and with regard to the micromechanics of grain boundaries. On the side of numerical efficiency, the extension of a spectral method that, as an alternative to FEM, solves static equilibrium in periodic domains, i.e., representative volume elements, towards finite strains and arbitrary material constitutive laws indicates prospective speed-ups by one to two orders of magnitude.

The Nature of Laves Phases –
An Inter-Institutional Research Initiative of the Max Planck Society

F. Stein, O. Prymak, S. Voß, C. He, M. Palm, G. Frommeyer, D. Raabe

In 2006, the inter-institutional research initiative "The Nature of Laves Phases" was established as an interdisciplinary project among four Max Planck institutes. The MPI for Chemical Physics of Solids in Dresden, MPI for Metal Research and MPI for Solid State Research, both in Stuttgart, and the MPI für Eisenforschung GmbH are closely collaborating within this research initiative to perform experimental and theoretical, interdisciplinary investigations of complex intermetallic phases. The physical metallurgy of intermetallic phases such as the Laves phases is much more complex than that of other established alloys, but has to be understood in greater detail as these phases are promising candidates for the design of new metallic materials with the intermetallic phase as the matrix phase or as hardening precipitates, e.g. in damage-tolerant high-strength steels for light-weight engineering applications or high-temperature alloys with good creep resistance for CO_2-reducing energy converting technologies.

The ternary systems TM–Nb–Al (TM = Cr, Fe, Co) were chosen as model systems as their phase diagrams are characterized by extended phase fields of the cubic C15 and the hexagonal C14 and C36 Laves phases. Within the last two years, isothermal sections of the ternary phase diagrams were determined by detailed experimental investigations of equilibrated alloys heat-treated at temperatures ranging from 800 to 1450°C [1-4]. The crucial role of structural defects and distortions in the crystal lattices of the different Laves phase polytypes has been investigated both experimentally and by quantum-mechanical calculations [5]. Site occupancies of the different atom types in the ternary C14 Laves phase lattice were studied by Rietveld refinements of powder XRD patterns in order to discuss the stability of the hexagonal vs. cubic crystal structures [1,4]. Based on the experimentally obtained phase equilibria and invariant reaction temperatures, isothermal sections of the ternary phase diagrams can be thermodynamically modelled by the CALPHAD method for experimentally inaccessible temperatures enabling a detailed discussion of stability and transformation of the different Laves phase polytypes [6,7].

Another topic is the mechanical behaviour of Laves phases in dependence on structure and composition (see also p. 93). For mechanical testing, bulk single-phase bars (15 mm in diameter and at least 120 mm in length) with stoichiometric and various non-stoichiometric compositions were synthesized by a modified levitation melting technique [8]. Deviations from the stoichiometric composition are compensated by defects of the anti-site atom type in case of transition metal Laves phases. Whereas the introduction of defects in metals and certain intermetallic phases like the well-investigated B2 compounds FeAl and NiAl typically results in a hardening of the material, yield strength and hardness measurements of single-phase Laves phase alloys indicate that significant defect softening takes place when lowering the Nb content from the stoichiometric composition [9].

More information on the research initiative "The Nature of Laves Phases" can be found on the project website http://Laves.mpie.de.
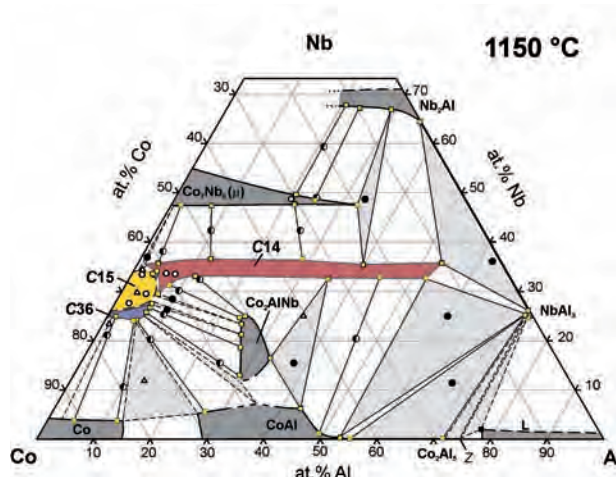
Isothermal section of the ternary Co-Nb-Al phase diagram showing the extended phase fields of the C14, C15 and C36 Laves phases [1].

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THE INSTITUTE

Ab initio Description of Iron and Steel (ADIS): An International Workshop Series

T. Hickel, M. Friák, J. von Pezold, J. Neugebauer

Since the opening of the Department of Computational Materials Design in 2005, the vision of a solely computer-based materials design (with steels particularly in mind) using *ab initio* methods became one of the driving forces of active research at the MPIE. It is further the fundamental idea behind the SFB "Stahl – *ab initio*" (p. 29) and ICAMS (p. 28), which are both strongly linked to the MPIE activities. Being a rapidly developing and highly competitive and rewarding field of research, several other research groups worldwide follow a similar vision. However, the complexity of realistic iron-based materials with respect to chemical, magnetic and micro-structure is a challenge for every *ab initio* approach. Consequently, there is not just a single well paved road of method development. Instead – to have success – a wide array of approaches and algorithms needs

to be implemented, evaluated, and carefully checked with respect to their predictive power. This challenge is well appreciated in the materials science community and can only be tackled in a combined multi-disciplinary effort.

To catalyze this effort the Department of Computational Materials Design established a series of international scientific seminars starting in 2006. The "*Ab initio* Description of Iron and Steels (ADIS)" workshop series provides the required platform for the leading experts in *ab initio* metals research to discuss and exchange recent results and scientific developments. The meetings 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). In October 2010 already the third seminar of the ADIS series has been performed. 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 ADIS2006, for example, was mainly about the combination of density functional theory with thermodynamic concepts. The focus of ADIS2008 was on approaches to complex magnetic phenomena and the latest meeting was devoted to mechanical properties, including dislocation related mechanisms. This change of specific focus resulted in a stimulating and highly productive exchange of experts, who – often coming from communities with little or no overlap – quickly grasped the chances of working together in such an interdisciplinary field. The series is now an established and integral part in the community.

PART II.

THE DEPARTMENTS

(in alphabetical order)

T H E

D E P A R T M E N T S

Department of Computational Materials Design

J. Neugebauer

Scientific Concept

The objective of the department "Computational Materials Design" is the development, implementation and application of quantum mechanical based simulation techniques to reliably predict properties and mechanisms in modern engineering materials. A major challenge in developing accurate and at the same time numerically feasible simulation techniques is the structural and chemical complexity inherent to virtually all materials of technological interest. This complexity is a direct consequence of the hierarchical nature in length and time scale, but also in the physical mechanisms involved and must be included to predict and understand materials properties relevant to the engineer.

The inherent complexity renders any direct brute force quantum mechanical approach unfeasible. Therefore, well controlled approximations and efficient numerical formulations are of utmost importance both at the quantum mechanical level – a direct solution of the exact Schrödinger equation is out of reach for any realistic system – as well as for bridging the gap between the electronic/atomistic and the macroscopic/engineering scale. Consequently, the department follows three major research routes:

(i) Analyze and quantify the accuracy of presently available ab initio techniques

In any *ab initio* based multiscale scheme the finally achievable accuracy will be limited to the one at the most fundamental (*ab initio*) scale, since the numbers generated at this level enter all subsequent higher levels. For density functional theory, which is the dominant *ab initio* technique employed for materials science questions, the one and only not systematically improvable approximation is the choice of the exchange-correlation (xc) functional. All other approximations at this level are controllable and can be made arbitrarily small, however, at the price of rapidly increasing computational costs. By carefully analyzing the underlying physics we were able to systematically develop numerical approaches that guarantee an accuracy that is only limited by the accuracy in the xc-functional. To accomplish this aim a completely new level of accuracy had to be achieved with error bars being one to two orders

of magnitude smaller (i.e. with errors in the total energy of often 1 meV and below) than what has been attempted in most previous studies. Examples are given in the highlight on p. 131 and in the group reports of T. Hickel (computation of thermodynamic quantities at finite temperatures) and C. Freysoldt (description of point defects in a supercell approach). The availability of these approaches helped not only to address the question of accuracy, but opened completely new research routes to address long standing fundamental materials science questions that were out of reach for existing theoretical and experimental tools [1,2], to unravel hitherto not discovered relationships [3,4], or to systematically test the reliability of commonly employed approximations [5]. Often, these results lead to a complete revision of well established concepts (such as e.g. the neglect of spin quantization in computing thermodynamic properties) thus initiating the development of a new set of simulation strategies.

(ii) Bridging the gap between quantum mechanical and engineering scale

While the quantum mechanical calculations provide an important first step in the multiscale hierarchy, the calculation of the relevant properties on the engineering scale requires in most cases additional simulation techniques. To be more specific, the *ab initio* codes do not allow to directly compute the various excitation mechanisms entering the free energy (such as anharmonic contributions or finite temperature magnetism), properties of polycrystalline and/or multiphase materials or fracture mechanisms to name only a few. In the last two years we have therefore acquired expertise in a wide range of simulation techniques helping to overcome parts of the scaling gaps. Examples are advanced molecular dynamics methods to efficiently sample high-dimensional configuration spaces [1,6], various flavors of statistical approaches such as kinetic Monte Carlo to access long time scales as relevant for diffusion [7] or spin Quantum Monte Carlo to describe magnetic excitations [3], microscopic elasticity theory to describe long range elastic interactions in martensitic transitions [8,9], cluster expansion [10] and the concept of quasi random

structures (SQS) [11] to include chemical alloys, or various homogenization schemes [12-14]. For many of these techniques we had to develop own computer programs, often implemented in our highly modular and object oriented SPHInX multiscale library [15,36]. Having this set of state-of-the-art tools available allowed the department to design optimum multiscale strategies for a wide range of problems: Concurrent approaches where parameters are passed through all scale (e.g. to identify mechanisms behind delayed fracture [6]), scale jumping approaches where the quantum mechanical information can be directly used at the macroscopic scale [4,12-14,16, and the highlight on p. 133], or multi-physics approaches to predict quantities that intrinsically connect several physical mechanisms (such as e.g. free energies consisting of vibronic, electronic, and magnetic excitation mechanisms) [1,3,5,9,17].

(iii) Translating industry-relevant science questions into formulations accessible by ab initio

The translation of industry relevant materials science questions into models that are accessible by *ab initio* based multiscale approaches often turns out to be highly non-trivial and challenging, requiring in many cases the exploration and development of methodological concepts. Examples concern the understanding of the microscopic origins causing delayed fracture (H embrittlement) in modern high-strength steels [6], identifying correlations (mechanism maps) between chemical composition and active deformation mechanisms in TWIP/TRIP steels [10], or preventing oxidation/corrosion mechanisms at metal surfaces [1]. In close collaboration with industrial partners and experimental groups and often stimulated by concrete and pressing technological bottlenecks we explored and developed a wide range of new methodologies. Challenges we had to face were related to incomplete experimental knowledge concerning microstructure and/or local chemical composition in complex engineering materials, noise in the experimental data particularly when going to extreme conditions such as near the melting temperature, but also limitations in the principal accuracy of present days *ab initio* techniques. A substantial amount of work had therefore been devoted to identify and carefully quantify sensitivity and error bars and to develop robust schemes allowing to obtain qualitative insight and numerical models even when working with noisy input data. Examples are our high precision tools to predict thermodynamic data (e.g. heat capacities) with an accuracy well beyond experimental scatter providing a completely new route to reassess experimental data [1,17,18], or our "divide and conquer" approaches that seamlessly connect well established empirical approaches such as e.g. CALPHAD that provides bulk free energies with an accuracy presently not achievable by any available *ab initio* technique with

quantum mechanical concepts to compute critical engineering parameters such as e.g. stacking fault energies with an accuracy well beyond what was previously possible (see p. 129). Although these developments are still in their first stages, the physical insight obtained already now indicates the potential these methods will have in the future.

While the development of these major research routes had been largely separated in the previous two periods and individually pushed by the scientific groups in the department, the tremendous progress made in this period opened the possibility to connect these activities. As outlined in the group reports and highlight articles, this opportunity has been intensively used resulting in many new inter-group and inter-departmental activities yet strengthening at the same time the individual scientific expertise in each group.

The availability of this large set of actively developed, cutting edge simulation tools for the multi-scale study of materials properties allowed us to address a wide range of materials science questions with the main focus on steel but also to cover key technological problems in semiconductor lighting, photovoltaics, nanostructures, and bio-inspired materials. Many of the publications received special attention from the journal editors such as the label "editors choice" [19-21], the new level of accuracy in *ab initio* computed thermodynamic properties achieved [1] was commented by a viewpoint article with the provocative title "Turn off the lab furnace and boot up the mainframe" [2], and members of the department received numerous invitations and keynote talks. Also, members of the department received prestigious awards such as C. Freysoldt, who received the Psi-k Volker Heine Young Investigator Award for "excellence in research involving electronic structure calculations" at the largest electronic structure conference taking place only every 5 years, or B. Grabowski who became a member in the DFG "Nachwuchsakademie" together with grant money to perform his own research.

The department was also actively involved in shaping and developing this new field by organizing and co-organizing international workshops such as the ADIS2008 and ADIS2010 meeting (see p. 35) and "Excitement in Magnetism" all at Ringberg Castle, a CECAM Summer School in San Sebastian on "Computational Materials Sciences" and symposia at key conferences e.g. on "Multiphysics Modeling in Materials Design" at the 2009 MRS meeting in Boston, on "Structural Materials and Steels" jointly with the DGM at the 2010 Spring DPG meeting in Regensburg, on "Alloy theory" at the Psi-k 2010 electronic structure conference in Berlin, on "Multi-Scale Computational Materials Design of Structural Materials" at the ASIA Steel conference 2009 in Korea, or on "*Ab initio* modeling" at the EUROMAT in Glasgow. The strong activities in developing new

Fig. 1: *B. Grabowski (right) explains the shape-memory effect at one of the highlight stations to visitors of the MPIE at the open day event.*

simulation techniques and in identifying novel areas for applying these methods stimulated a large number of national and international collaborations and helped attracting a large number of research funds. In this period, important research collaborations could be initiated with leading research institutions on steel research in the USA, Sweden, Russia, Korea, and China by exchanging scientists, organizing joint meetings or jointly applying for funding. Major projects the department is involved in are the SFB "Steel – *ab initio*" (see p. 29), DFG focused projects and research groups e.g. on magnetic shape memory alloys and bio-nanocomposites, several BMBF (federal ministry of education and research) projects on novel high-temperature steels (Ferrit950), on high-brightness energy efficient light emitters (VEKTRA), and on

photovoltaics (EPR-Solar), an international RFCS project on hydrogen embrittlement (HYDROMICROS) and EC projects on nitride semiconductors.

Strong links and collaborations have been established with the recently founded **Interdisciplinary Center of Advanced Materials Simulations (ICAMS)** at the University of Bochum (see p. 28). The department is actively involved with the center by heading the Advanced Study Group "Modeling" (director – Prof. J. Neugebauer, speaker – T. Hickel) and establishing several joint projects on key topics such as e.g. H embrittlement or the *ab initio* description of finite temperature magnetism. To foster strong collaborations and interaction between the scientists in the two institutions from the very beginning several joint workshops have been organized by our department (Ebernburg 2009, Imst 2010) or by ICAMS (Attendorn 2010).

Members of the department were also highly active in **training young scientists and students**. Lectures on various issues of computational materials science were given at the University of Bochum and the RWTH-Aachen to engineers and physicists. In the reporting period one Bachelor, three Master and six PhD theses have been successfully finished. The department also actively participated at the open day event (p. 190) showing with great enthusiasm to the public how basic research can help to address "hot" technological questions (Fig. 1). Due to the large increase in third party funding the department grew substantially totaling in more than 30 scientists (Fig. 2). To ensure sufficient computer power for such a large group the high-performance computer cluster had to be constantly upgraded (see p. 24).
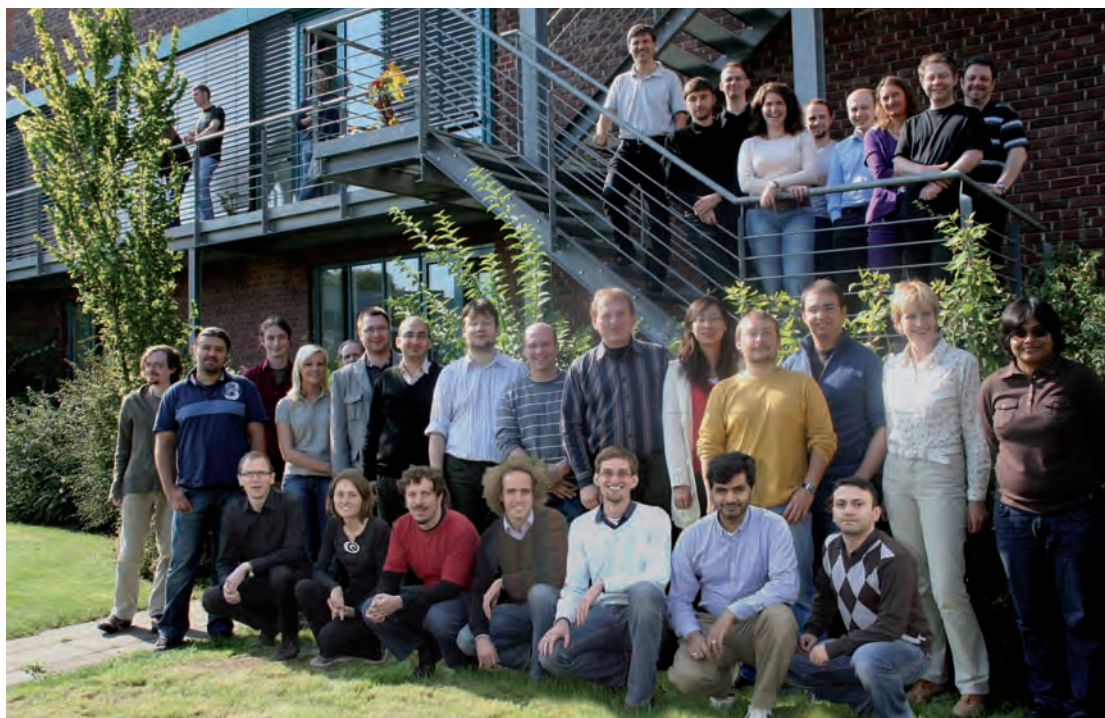

Fig. 2: *Members of the department (Summer 2009).*

The growth of the department, the opening of new research topics, and the leave of key personal required changes in the group structure. The head of the Algorithmic Design and Modeling group and head of the computer center, S. Boeck, used his rich expertise acquired in setting up supercomputer centers and in developing large scale scientific software projects to found his own company "Gemmantics IT Consulting". As a consultant, he will continue to assist the department with setting up high performance computer clusters. Due to his new position, the coordination of the development of our multiscale library SPHInX has been transferred to C. Freysoldt who has been also one of the key developers over the last years (see p. 48).

The large methodological progress achieved allows us to tackle critical metallurgical questions that were out of reach a few years ago. To provide a platform for these activities the former group of S. Boeck has been replaced by the group "Precipitation and Kinetics" headed by A. Dick (see p. 17). The aim of this group is the development of multiscale techniques that allow an accurate description of kinetic processes in the nucleation and time evolution of precipitates and of extended defects. Collaboration with theoretical and experimental groups from other departments (e.g., experimental characterization of precipitate patterns with the atom probe tomography group, P. Choi), as well as other institutions (phase field simulations using multi-component multi-phase phase field (Prof. I. Steinbach, ICAMS, Germany), precipitation kinetics (Prof. E. Kozeschnik, Vienna University of Technology, Austria)) will strengthen the expertise of this group.

The ability of the department to link the electronic scale to actual technological questions will be also significantly strengthened by another key appointment. In August 2010 R. Spatschek, an internationally renowned expert on phase field and mesoscale simulations, accepted a W2 group head position and initiated a new group "Mesoscale Simulations" (see p. 20). This group will be also instrumental to further strengthen the link to the macroscale simulations in the department of Prof. Raabe and to open additional connections to the mesoscale activities at ICAMS. Both new research groups will significantly strengthen existing activities in the department by opening new links between the *ab initio* thermodynamics activities (groups "Computational phase studies", T. Hickel, and "*Ab initio* thermodynamcs", M. Friák) and microstructure characterization ("Microstructure" group headed by L. Lymperakis).

In the following a brief description of the activities and recent developments of the scientific groups is given.

Scientific Groups

Computational Phase Studies (T. Hickel)

The research in the group "Computational Phase Studies" is devoted to the physics of (meta)stable thermodynamic phases in metals and transitions between them. A major aim is the prediction of thermodynamic bulk phase diagrams, due to their direct relation to many technologically relevant properties and processes in metals. The group aims at a full *ab initio* derivation of these properties, mainly making use of density functional theory (DFT). In this context, many of the methods developed by the group in the last period have been extended, applied to advanced material systems, and supplemented by additional tools. This applies in particular to the following fields of research:

- The continuous improvement of *ab initio* based methods to calculate the relevant contributions to the free energy of metals, their application to industrially important materials, and the combination of the results with thermodynamic databases.

- The description and prediction of temperature and stress induced phase transitions and/or structural changes in shape memory alloys, steels and related materials.

- The energetics and kinetics of alloying elements, impurities and defects, and their relevance for embrittlement phenomena, precipitation and ductility of materials.

In the following some of the key activities in these fields will be briefly discussed and resulting collaborations will be mentioned in selected cases.

In order to **derive free energies from first principles**, one needs to combine DFT with thermodynamic concepts. In previous works we have particularly concentrated on the performance of the quasiharmonic approximation, including electronic excitations and achieved remarkable agreement with experimental data for non-magnetic unary metals. These concepts have been extended (B. Grabowski) towards the consideration of anharmonic lattice
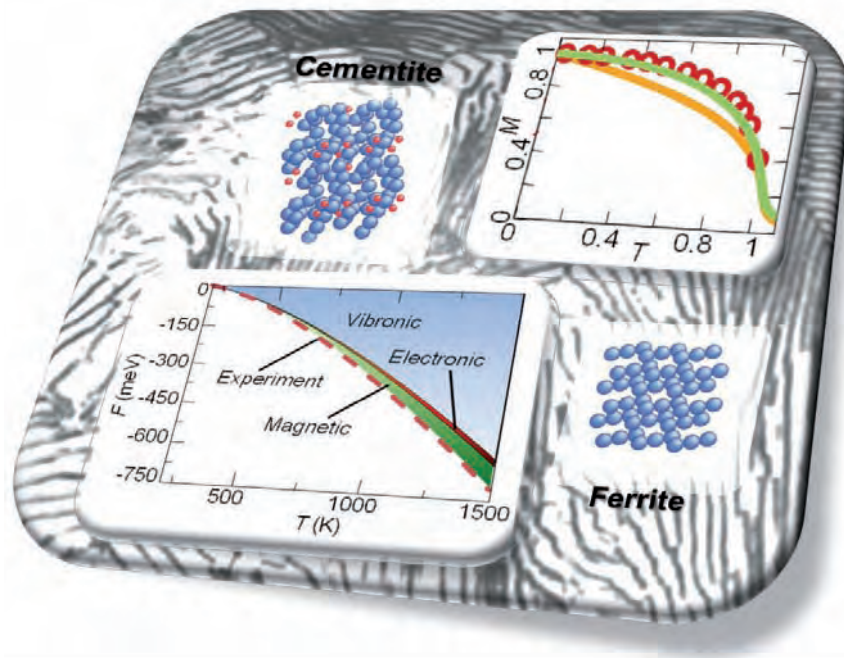
Fig. 3: *Thermodynamic properties of steels derived from first principles. In the background the pearlitic microstructure of a 0.8%C steel containing ferrite and cementite phases is shown. Upper right inset: The experimental magnetization of ferrite (red symbols) is compared with our Quantum Monte Carlo approach (green line). Lower left inset: The free energy of cementite (experiment: dashed line) is compared with our combined* ab initio *approach including contributions from vibronic, electronic and magnetic excitations.*

vibrations, of entropically stabilized vacancies [1,35], and of thermodynamically unstable phases [22]. The availability of such a large set of precise tools to study free energy contributions is a characteristic feature of the group and enabled us to address and solve a wide array of materials science questions. Many of our contributions, such as the one on the (for a long time highly controversially discussed) question about the dominant free energy contributions of a material close to the melting temperature [1], received considerable attention in the community [2]. Presently the developed methods are generalized – in a combined effort with CALPHAD evaluations – to chemical alloys. For the prototype system of Al alloys (A. Glensk), relevant for light-weight materials design, this work is performed within a DFG project with several partners in Germany.

For steels, the **magnetic excitations** form the most challenging contribution for a computational materials design, both with respect to methodological and numerical concepts, due the long range interactions and spin-quantization. After having derived analytical approaches to obtain the magnetic heat capacity of bcc iron up to the Curie temperature [5], several schemes based on classical and quantum Monte Carlo (MC) simulations have recently been developed, carefully explored [3] and finally used (F. Körmann). The discovered universality of the new MC-based approaches made an application to

various magnetic phases including the paramagnetic state (relevant e.g. for many austenitic steels) possible. The methods have successfully been applied to various magnetic materials [23], including relevant phases in steels such as e.g. cementite [18], Fig. 3. Whereas the experimental investigation of its heat capacity resulted in a large scatter, our fully *ab initio* approach allowed to identify the correct temperature trends [17], nicely demonstrating the power of the approach. Recently, in a joint project with the RWTH Aachen we succeeded in combining the *ab initio* computed magnetic free energies with CALPHAD assessments (see p. 129).

For the simulation of **martensitic phase transitions** in the magnetic shape memory alloy Ni_2MnGa (A. Al-Zubi), it turned out again that the consideration of temperature dependent magnetism is decisive. Only by considering the delicate interplay of vibrational and magnetic excitations we were able to correctly describe the sophisticated sequence of phase transitions in this alloy [22]. We have now succeeded in using these methods for a prediction of chemical trends in the phase stabilities (Fig. 4, next page). Our part within a large scale DFG project on this subject has recently been extended by two years.

High manganese steels form another class of materials, where martensitic phase transitions influence the plastic behavior considerably. Depending
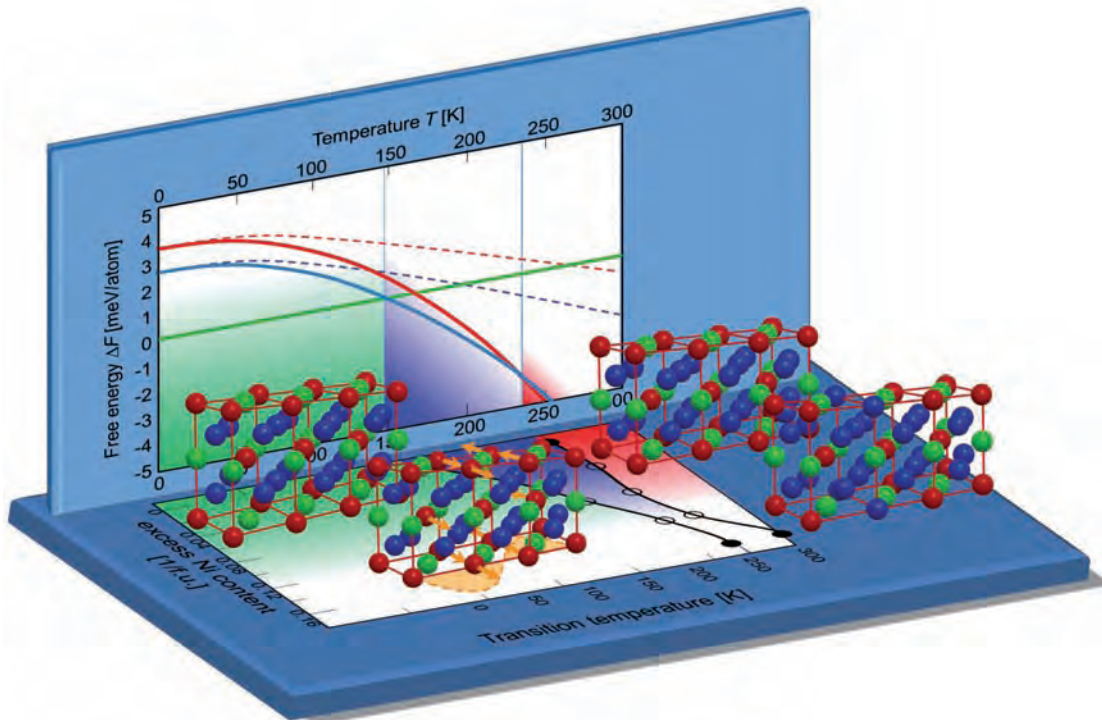
Fig. 4: Ab initio *prediction of the phase diagram of $Ni_{2+x}Mn_{1-x}Ga$ [22]. Upper panel: The free energies of the martensite (green line - reference), austenite (red line) and premartensite (blue line) have been determined for different values of x (here: x=0). Only the solid lines take magnetic excitations into account, whereas this is not the case for the dashed lines. Lower panel: The transition temperatures derived from the intersections of the free energies are plotted as a function of x. The colored regions in the phase diagram indicate the thermodynamic stability of the respective phases. The crystals structures (blue: Ni, red: Mn, green: Ga) belong to the different phases and chemical compositions.*

on the stacking fault energy (SFE), the transition might compete with the twinning of the material under stress. We (A. Dick, A. Abbasi) have therefore performed intensive investigations on chemical and thermodynamic trends for the SFE [10,37], gaining remarkable insights into its dependence on temperature, pressure and carbon content. Within the collaborative research center SFB 761 "Stahl – *ab initio*" our calculations where in particular helpful to systematically determine parameters in empirical approaches to the SFE, which one would need to guess otherwise (see p. 129).

In order to consider **diffusion processes on an atomistic scale**, as for instance done for hydrogen, kinetic Monte Carlo simulations in combination with transition state theory are typically used. Apart from the hydrogen problem, we have used this tool for several other applications in the group. For example, self-diffusion is systematically investigated in Fe-Al (N. Sandschneider), incorporating sophisticated jump cycles (Fig. 5) and combining it with large scale simulations in a joint project with a Chinese partner. Another example are diffusion processes related to precipitate formation in steels (N. Tillack), which are compared with atom probe experiments at

the MPIE (see p. 103). Some of these aspects will be continued more intensively in the newly founded group "Precipitation and Kinetics", headed by A. Dick.

The effect of hydrogen in particular in the context of embrittlement mechanisms, is a key topic to the entire department. In this group we therefore made intensive and systematic investigations on the solubility and diffusion of hydrogen in metals [24] and steels [7], including also the effect of superabundant vacancy formation due to hydrogen (R. Nazarov, U. Aydin, N. Hamidi) [25, see also highlight on p. 113]. These activities resulted in an RFCS project on the relation between microstructure and hydrogen embrittlement, coordinated by the head of the group (T. Hickel).

Ab initio Thermodynamics (M. Friák)

The group is focused on the development and application of theoretical approaches allowing scale-bridging simulations of materials properties. Employing them, a theory-guided design of materials intended for specific industrial applications is per-
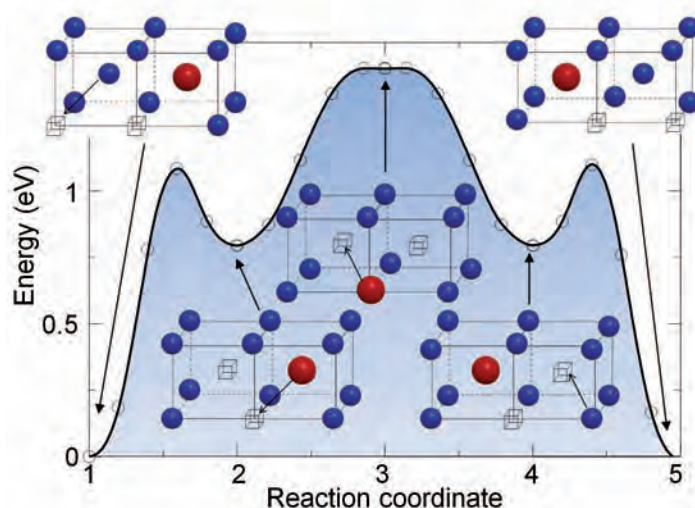
Fig. 5: *Triple defect mechanism for the self-diffusion in FeAl. The minimum energy path has been determined using the nudged elastic band method. The relevant jump processes are indicated by arrows in the crystal structures. Red spheres correspond to Al, blue spheres to Fe.*

formed (see highlight on p. 133). Due to the complex multi-scale nature of most of the studied problems, the applied strategies are intrinsically multi-disciplinary and multi-methodological. Cooperating closely with scientists from different fields from both inside and outside the MPIE, one of the key objectives of the group is the development of *ab initio* based theoretical/computational tools that provide data not accessible by experiment and a systematic screening and design of alloys with tailored macroscopic elastic properties.

The **range of materials** studied in the group covers single-phase and double-phase metallic alloys as well as multi-phase hierarchically organized bio-composites. Aiming at exploring new metallurgical concepts and extending the limits of materials design, novel alloys with extreme but technologically highly relevant properties were searched for. For example, a systematic search for an optimum composition of biocompatible Ti-Nb implant alloys that matches the elasticity of human bones resulted in nearly two-fold reduction of the Young's modulus [26].

Using a similar concept we presently study **dual-phase high-strength ductile eutectic Fe-Ti alloys** within a DFG-funded project performing *ab initio* calculations (L.-F. Zhu, see p. 133), phase-field modelling (Prof. H. Emmerich, Bayreuth University), and experimental techniques (Prof. J. Eckert, Institute for Complex Materials at the Leibniz-Institute for Solid State and Materials Research in Dresden).

Quantum mechanical calculations have also been used to provide key parameters for classical **solid-solution strengthening** concepts applied to Al in order to increase its strength and obtain a deeper

understanding of fundamental processes responsible for such a strengthening (in a cooperation with J. von Pezold, T. Hickel, D. Ma and Prof. D. Raabe). Applying this strategy helped not only to identify alloys with tailored properties but also to reveal fundamental materials-design limitations. Examples are Mg-Li-base alloys where a simultaneous increase of stiffness and ductility was shown to be principally impossible [4,12,13,27] (see also p. 133).

A strong focus has been also on **iron-based materials**, where e.g. the long-range elastic inter-actions in a ferritic matrix containing C interstitials have been studied combining microscopic elasticity theory (MET) with atomistic models (A. Udyansky and J. von Pezold). This novel multiscale approach provided a deeper understanding of the role played by C in phase transitions between ferritic, martensitic and austenitic steels [9,8]. Aiming at structural properties, the origin of the volume-compositional anomaly in Fe-Al alloys has been identified and linked to magneto-volume effects [28]. Extending the Fe-Al alloys to ternary systems, the polycrystalline elastic properties of Fe_3Al-based materials were studied in a combined theoretical and experimental approach [16,29] and in close cooperation with experimentalists from the other departments (J. Deges, F. Stein, M. Palm, R. Krein and Prof. G. Frommeyer).

Inter-departmental research is currently also applied to **high-temperature materials**. These materials are often strengthened by various precipitates such as Laves phases or e.g. transition metal disilicides ($TMSi_2$). A BMBF-funded project (Ferrit 950) links the theoretical and experimental expertise of this group (F. Liot) with that of the groups of T. Hickel, of S.
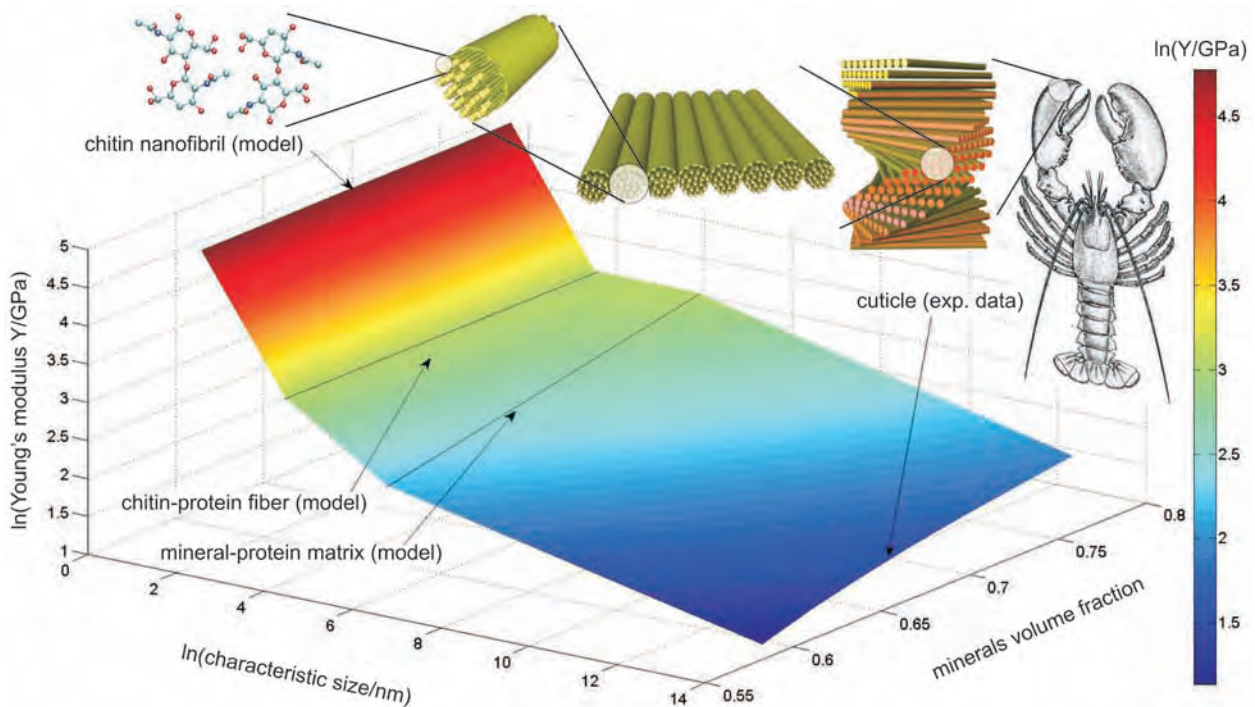
Fig. 6: *Scale-propagation of the Young's modulus through the hierarchical structure of lobster cuticle [31]. The log-log dependence of Young's modulus as a function of the characteristic size is visualized together with its dependence on the volumetric fraction of minerals. Each length-scale (from nano-meters to centimeters) is schematically accompanied by a characteristic element of the hierarchical structure governing the elasticity.*

Weber at the Ruhr University Bochum, and also with in-house experimental activities (S. Voß, F. Stein, and M. Palm; see p. 93). Research on simulating the behaviour of $TMSi_2$ under extreme loading conditions is performed together with Prof. M. Šob from Masaryk University, Czech Republic [30].

The tools originally developed to study metallic alloys could be also successfully employed to study

the elasticity of **hierarchically-organized biological nano-composites**. One example is the study of the cuticle of a lobster in a joint research project with the "Microstructure" group, and the department of Prof. Raabe. Applying the novel approach it became possible to describe the evolution of the mechanical properties all the way from the atomistic level up to the macroscale (Fig. 6) providing unique insight into how nature realizes enormous stability with
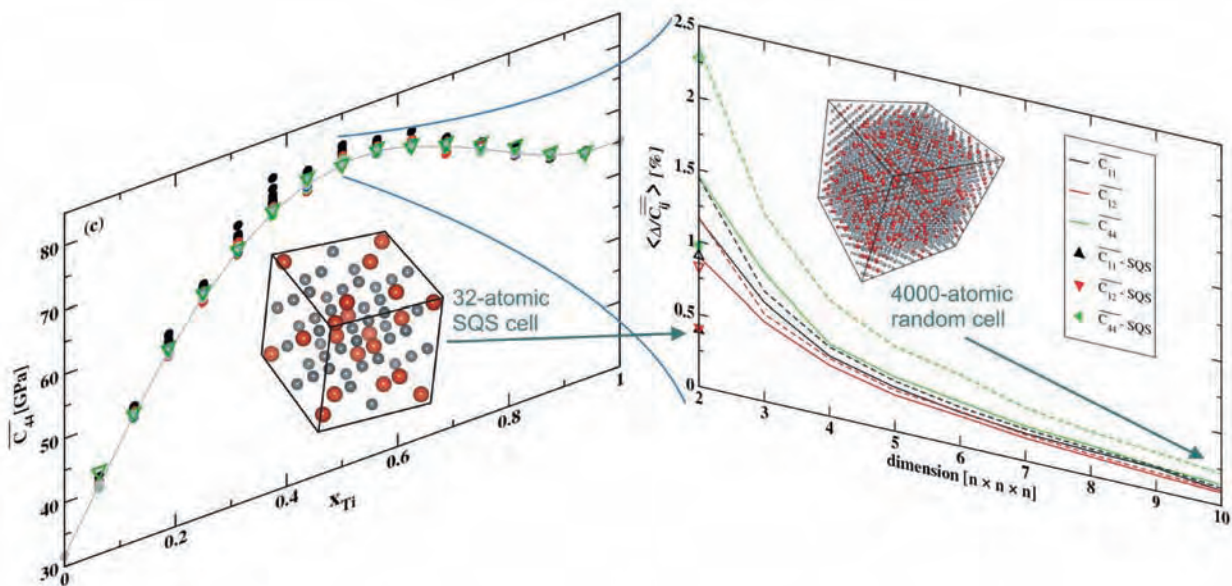

Fig. 7: Ab initio *predicted compositional dependence of the C_{44} elastic constant in Ti-Al face-centered cubic alloys obtained using 32-atomic special quasi-random structures (left) that has virtually an identical performance as a fully size-converged conventional 4000-atom super-cell [11] (right).*
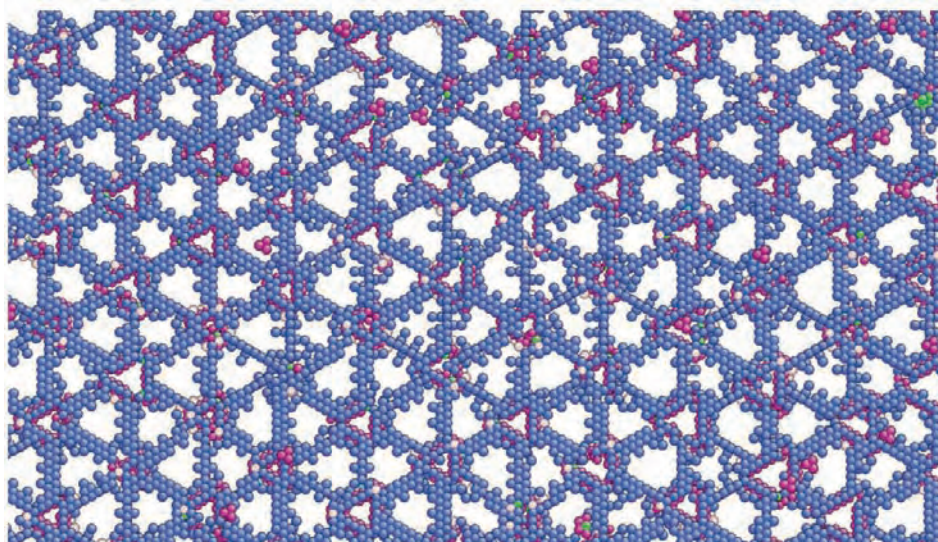
Fig. 8: *Low coordinated atoms at the Cu_3Au/Au interface. The interfacial strain relaxes by forming a hexagonal network of misfit dislocations.*

light-weight components [31]. The methodology is presently extended (P. Elstnerová) to calcite based composites [32] in a cooperation with the groups of T. Hickel, Prof. S. Hild from Johannes Kepler University Linz and A. Zigler from the University in Ulm.

The methodological aspects of the various multi-physics and multi-scale schemes were supplemented by carefully analyzing **error-propagation and numerical robustness** of different homogenization schemes [13], combining *ab initio* determined elastic constants with Finite Element Method (FEM) simulations [14] (in a close cooperation with F. Roters, D. Ma, and Prof. D. Raabe), or extending the concept of special quasi-random structures (SQS) to calculations of elastic constants of alloys (Fig. 7, [11]) (together with J. von Pezold and A. Dick).

Microstructure (L. Lymperakis)

The focus of the microstructure group is on the atomistic description of the mechanisms underlying static properties and dynamic evolution. The group expertise covers the topics of extended defects, interfaces, and surfaces. The aim of the group is to (i) provide an atomic-scale understanding and quantify the interplay between the atomistic mechanisms and the properties of the extended defects such as cohesion and mobility of interfaces and electronic structure of dislocations and (ii) to identify kinetic pathways in terms of surface engineering which allow for a full control over the morphology and the microstructure of epitaxially grown materials.

Electrochemical dealloying of metallic alloys can be regarded as a detrimental (wet) corrosion process related e.g. to stress corrosion cracking. Noble metal alloys like Ag-Au or Cu-Au constitute model systems and are investigated to gain basic understanding of corrosion processes. In collaboration with F. Renner from the Department of Interface Chemistry and Surface Engineering, we investigate the microstructure of the Cu_3Au/Au heterophase interface formed during the dealloying process of Cu_3Au surface. In order to gather a deeper and on-atomic-scale understanding of the strain relaxation mechanisms underlying the Cu_3Au/Au system we performed large scale calculations using Embedded Atom Method (EAM) potentials (Fig. 8). Our calculations revealed how long range surface strain affects the initial stages of interface formation and gives rise to a complex and hitherto not understood network of extended defects [40].

Novel nanostructures such as nanowires, nanobelts, and nanocolumns constitute key features in the design of novel materials with applications in catalysis, hydrogen storage, sensorics, and nanoelectronics. In order to fully exploit the unique characteristic of these nanomaterials it is critical to understand and identify the atomistic mechanisms underlying their growth. We have therefore developed a novel hierarchical approach which combines *ab initio* kinetics and surface thermodynamics with mesoscale finite difference calculations [21]. This approach allows to incorporate realistic growth geometries and conditions (Fig. 9, next page) and provides a full qualitative and even quantitative description of the growth of such nanowires (see p. 135). The aforementioned hierarchical model constitutes a novel tool in designing and optimizing the growth and the properties of the nanostructures.
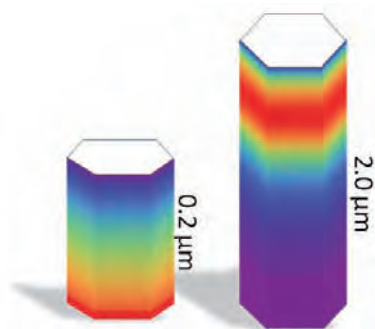
Fig. 9: *Simulated adatom density distribution on the side facets of nanowires at realistic growth conditions using* ab initio *computed total energy surfaces. The nanowires shown here have identical cross sections but vary in length by an order of magnitude.*

Group III-Nitride semiconductors are materials widely used for optoelectronic applications such as Solid State Lighting (SSL) based on Light Emitting Diodes (LEDs) and Laser Diodes (LDs) as well as for high temperature and high power microelectronic devices and are of special interest for the automobile industry. The group is currently active in three projects within the field of III-Nitrides: (i) Electronic structure of (0001) GaN surfaces: Towards functionalizing the III-Nitride surfaces for biological and chemical sensing applications, in collaboration with the Institut für Physik and Institut für Mikro- und Nanotechnologien (TU Ilmenau, Germany)**,** (ii) *ab initio* based surface phase diagrams of novel semipolar planes, in collaboration with the electron microscopy group of the Aristotle University of Thessaloniki (Prof. Ph. Komninou), and (iii) electronic structure of screw dislocation in GaN: Formation of natural quantum wires, in collaboration with the "*Ab initio* thermodynamics group" and the Leibniz Institute for Crystal Growth (M. Albrecht), Berlin, Germany.

H-embrittlement of metals is a problem of both fundamental interest and huge technological impact, particularly due to its detrimental effects on high strength steels. Over the last two years we investigated in detail the Hydrogen Enhanced Local Plasticity (HELP) mechanism [6]. Using a multiscale approach combining *ab initio*, empirical potentials and kinetic Monte Carlo simulations we were able to demonstrate that H-H interactions within the metal matrix are of critical importance: Attractive H-H interactions give rise to the formation of hydride-like precipitates, while a Cottrell-like H atmosphere was observed in the absence of such interactions. As could be further shown the two H-phases have a very different effect on a dislocation. While in the latter case H screens the interaction between dislocations (eventually causing ductile fracture) only at very large bulk H concentrations (> 10 at.%), the presence of local hydrides makes this mechanism possible already at H concentrations that are more than two orders of magnitude lower.

The **mobility of grain boundaries** is of key importance for many technologically important processes, such as recrystallisation and grain growth. Despite extensive research over the last 20 years, the fundamental mechanisms and activation barriers for the migration of grain boundaries are still not fully understood. A careful analysis based on molecular dynamics (MD) studies of grain boundary mobilities, revealed systematic deficiencies in the generally used orientation-dependent driving force. We are therefore currently developing alternative, semi-local orientation measures, in order to effectively average out the effect of thermal noise on the applied driving forces (C. Race, J. von Pezold).

Defect Chemistry and Spectroscopy (C. Freysoldt)

The group "Defect Chemistry and Spectroscopy" 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 semiconducting and insulating materials. Computer simulations are a powerful tool to better understand the formation of point defects, their properties, and their role in modifying macroscopic material parameters. Major challenges in the simulation arise from (1) providing a reliable theoretical framework to accurately compute the defect energetics, notably the formation energy and electrically active transitions within the band gap of the material, (2) from linking the microscopic picture to a coarse-grained theory that is able to describe the experimentally relevant time and length-scale (scale bridging), and (3) from developing useful approaches for point defects in amorphous/glassy materials.

Multi-scale program library SPHInX: The group actively develops new methods, that render the calculations more efficient and more accurate, and implements them into our modular multi-scale program library SPHInX [15,19]. One such development is a novel method to systematically correct for electrostatic artifacts that are unavoidable in charged defect supercell calculations [20]. These corrections are particularly important for defects in oxides or nitrides [33] due to the weak screening in the material and the high charge states that may occur.

A major effort in the last two years has been the incorporation of the PAW method that overcomes transferability limitations of the plane-wave pseudo-potential approach without compromising the efficiency and accuracy control of plane-wave basis sets. This is achieved by augmenting each core region with
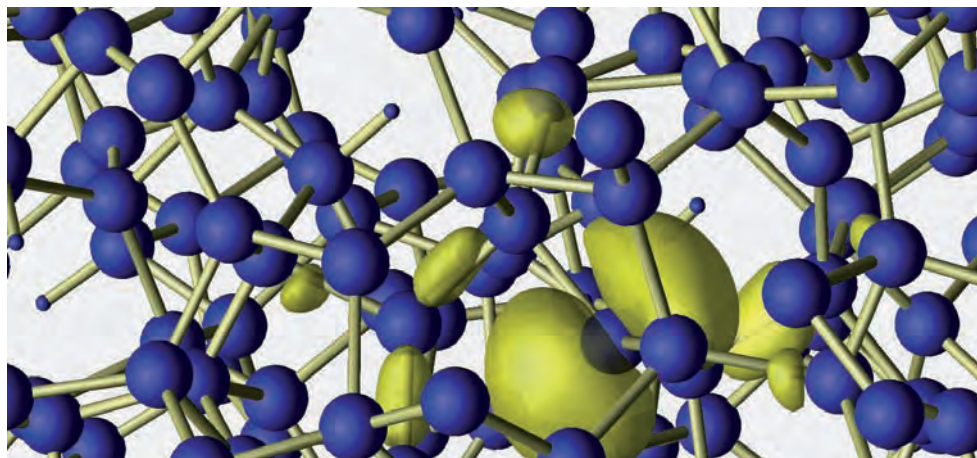
Fig. 10: *Spin density (yellow) of a dangling bond in hydrogenated amorphous silicon (large spheres: Si, small: H).*

an auxiliary basis set on a radial grid that is connected to the plane-wave representation with projection operators. Thanks to the object-oriented structure of the code [15], the initial implementation could be finished within a few months only (workload estimates from experienced developers were 1-3 years). Key features of our implementation are (1) systematic control over radial, angular, and plane-wave grid parameters, (2) analytic consistency between energy and gradients (which is critical to enable efficient convergence to the numerical limit), (3) possibility to read a variety of PAW potential formats (atompaw, ab init, vasp, cppaw), (4) an overall performance comparable to other state-of-the-art codes. The PAW method is an important step forward since it complements our method developments on other levels of the multi-scale hierarchy (e.g. UP-TILD). At present, we are working on including hybrid functionals such as PBE0 and HSE in the PAW approach, since it has been recently shown that they overcome the severe limitations of standard DFT to describe band gaps (and thus also any defect levels within the gap).

Development of *ab initio* tight binding basis sets: Even though point defects consist of a few atoms only, they may interact with the host material over length scales that are not amenable to *ab initio* methods. One such effect is the localization of electronic states of shallow defects that may extend over several nm. It is therefore crucial to employ coarse-grained theories, e.g. tight-binding, and develop strategies to parameterize them from accurate *ab initio* calculations (accuracy transfer). For this purpose, a systematic method was developed to generate atomic-orbital basis sets of a given size that optimally mimic a given plane-wave calculation (B. Lange). Tight-binding calculations based on these orbitals reproduce plane-wave band structures within a few meV at a fraction of the computational cost. The method also provides basis sets that

optimally describe point defects. The approach thus combines the computational efficiency of the tight-binding method with the reliability of plane-wave calculations.

Defects in amorphous crystals: Understanding the formation of point defects in amorphous materials is a methodological and conceptual challenge, since many important concepts (such as thermodynamic equilibrium or an enumeration of relevant defect structures) do not apply. For example, hydrogenated amorphous silicon (a-Si:H) is a low-cost alternative to crystalline silicon for solar cells, that lends itself to large-scale mass production of solar cells on steel bands or other substrates. A major disadvantage of a-Si:H is the light-induced degradation of the material, that is related to the creation of dangling-bond defects. This Staebler-Wronski effect is known for more than 30 years, but still not fully understood. As a strategy to understand the properties of the dangling bonds in a-Si:H, notably their EPR parameters measured by our experimental collaborators, systematic studies for well-defined model defects in crystalline silicon [34] were combined with supercell models of the amorphous structure (G. Pfanner). The crystalline models were essential to identify the structural and electronic effects active in the material. The a-Si:H simulations, on the other hand, revealed that the actual properties of the defect only arise in the amorphous matrix due to the large flexibility of combining structural motifs that cannot coexist in the crystalline material (Fig. 10).

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Research Projects in Progress

Computational Phase Studies

Abbasi, Dick, Hickel, Neugebauer: Chemical trends for the stacking fault energy of high-Mn steels

Al-Zubi, Hickel, Neugebauer (in collaboration with K.R.A. Ziebeck*, K.U. Neumann*, P. Entel**, W. Petry***, J. Neuhaus*** ((*Loughborough University, UK, **Univ. Duisburg-Essen, ***FRM-II Garching)): *Ab initio* investigation of temperature dependent effects in shape memory Heusler alloys

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

Dick, 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

Dick, Hickel, Neugebauer (in collaboration with S.V. Okatov, Yu.N. Gornostyrev, Ekaterinburg, Russia): 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*)*

Grabowski, Hickel, Neugebauer (in collaboration with J. Neuhaus, FRM-II Garching): *Ab initio* based modeling of thermodynamic properties of metals close to the melting point

Grabowski, Neugebauer: *Ab initio* Untersuchung von temperaturgetriebenen martensitischen Phasenübergängen: Fallstudie für Erdalkalimetalle

Körmann, Dick, Hickel, Neugebauer (in collaboration with B. Hallstedt, 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

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

Sandschneider, Hickel, Neugebauer (in collaboration with M. Rettenmayr*, X. Song** (*U Jena, **Beijing, China)): Thermodynamic properties of $SmCo_7$

Tillack, Hickel, Neugebauer, Dmitrieva, Raabe: *Ab initio* study of nano-precipitate nucleation and growth in ferritic steels

Microstructure

Lymperakis, Neugebauer: *Ab-initio* based growth simulations of novel nanostructures

Duff, Lymperakis, Neugebauer (in collaboration with Forschungsverbund Berlin and TOP-GAN, (Warsaw, Poland)): Surface engineered InGaN heterostructures on N-polar and nonpolar GaN-substrates for green light emitters, EU Marie Curie Actions—Industry-Academia Partnerships and Pathways (IAPP)

Lymperakis (in collaboration with M. Himmerlich* and S. Krischok** (*Institut für Physik and **Institut für Mikro- und Nanotechnologien, TU Ilmenau)): III-Nitride based sensing applications: Electronic properties of III-N surfaces,

Lymperakis (in collaboration with F. Renner, Department of Interface Chemistry and Surface Engineering): Atomistic investigation of selective dissolution

Lymperakis, Neugebauer (in collaboration with M. Albrecht, Leibniz Institute for Crystal Growth, Berlin): Electronic properties of screw dislocations in GaN

Lymperakis (in collaboration with Ph. Komninou and E. Kalesaki, Department of Physics, Aristotle University, Thessaloniki, Greece): Semipolar III-Nitride surfaces

Lymperakis (in collaboration with Ph. Komninou and E. Kalesaki, Department of Physics, Aristotle University, Thessaloniki, Greece): Nudged elastic band calculations on the mobility of special grain boundaries

Defect Chemistry and Spectroscopy

Lange, Freysoldt, Neugebauer: Electronic embedding of defects using optimized atomic orbitals

Lange, Freysoldt, Neugebauer: Doping limits of GaN:Mg

Mitra, Freysoldt, Neugebauer: Band offsets within GW theory

Pfanner, Freysoldt, Neugebauer: EPR parameters of the dangling bond in a-Si:H

Freysoldt, Neugebauer: Efficient implementation of hybrid functionals in the PAW method

Ab initio Thermodynamics

Friák, Neugebauer (in cooperation with D. Holec, Montanuniversität Leoben, Leoben, Austria): *Ab initio* study of Ni-Ti shape-memory alloys

Friák, Neugebauer (in collaboration with D. Legut* and M. Šob** (*Institute of Physics of Materials (IPM), Academy of Sciences of the Czech Republic, Brno, Czech Republic, **IPM and Masaryk University in Brno, Czech Republic)): Theoretical tensile strength of transition metal disilicides

Zhu, Friák, Neugebauer (in collaboration with J. Eckert* and H. Emmerich** (*IFW Dresden, **RWTH Aachen University)): Scale-bridging studies of the elastic contributions to nucleation and initial microstructure formation in the eutectic system Ti-Fe

Elstnerová, Friák, Hickel, Neugebauer, Fabritius, Raabe (in collaboration with A. Ziegler*, S. Hild** and S. Nikolov*** (*University of Ulm, **Johannes Kepler University Linz, Austria, ***Bulgarian Academy of Sciences): Crustacean skeletal elements: variations in the constructional morphology at different hierarchical levels

Liot, Friák, Hickel, Neugebauer (in collaboration with N. Nabiran*, S. Weber*, H. Hattendorf**, H.-H. Angermann***, B. Sahebkar#, D.M. Kirch##, G. Brückner##, T. Beck#*, B. Eckardt#*, B. Kuhn#* (*Ruhr University Bochum, **Fa. ThyssenKrupp VDM, ***Behr, #Benteler, ##ThyssenKrupp Nirosta, #*Research Center Jülich): Ferrit950

Siboni*, Hickel, Friák, Neugebauer, Raabe (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES)): Effect of interstitials on vacancy formation and mobility in metals

Mesoscale Simulations

Schulz, Spatschek (in collaboration with A. Karma, Northeastern University, Boston): Morphology of pine tree nanowires

Hüter, von Pezold, Spatschek, Neugebauer: Continuum modeling of hydrogen embrittlement

Spatschek (in collaboration with G. Boussinot, E. Brener and H. Müller-Krumbhaar, Forschungszentrum Jülich): Elastic effects on heterogeneous nucleation and microstructure formation

Spatschek (in collaboration with W. Guo and I. Steinbach, ICAMS, Ruhr-Universität Bochum): Multijunctions in phase field models

Spatschek (in collaboration with B. Eidel and I. Steinbach, ICAMS, Ruhr-Universität Bochum): Plastic effects on the kinetics of phase transformations

Spatschek: (in collaboration with E. Brener*, M. Fleck** and D. Pilipenko** (*Forschungszentrum Jülich, **Universität Bayreuth)): Continuum modeling of fracture

Precipitation and Kinetics

Hausmann, Dick, Neugebauer: Influence of the alloying elements on the thermodynamic properties of cementite precipitates

Dick, Neugebauer (in collaboration with Grornostyrev, Institute of Quantum Materials Science, Russia): Early stages of precipitation in maraging steels

Dick, Hickel, Neugebauer: Kinetics of the stacking faults formation, segregation and out-segregation of alloying elements on grain boundaries and stacking faults in high-Mn steels

T H E   D E P A R T M E N T S

Department of Interface Chemistry and Surface Engineering

M. Stratmann

Introduction

Over the last two years the Department of Interface Chemistry and Surface Engineering has undergone major personal changes. Dr. Achim Walter Hassel left the department and took over a Chair on Chemical Technology at the Johannes Kepler University in Linz; Alexander Blumenau left the department for an industrial position. As a consequence, two new groups could be established in the field of Electrocatalysis (Dr. Karl Mayrhofer) and Atomistic Modelling (Prof. Dr. Alexander Auer). Over the last four years, four out of five groups have been re-established with new group leaders significantly changing the scope of the department. The department now has a much stronger focus in electrochemistry dealing with fundamental electrochemical reactions in corrosion science and energy research, high throughput methods and the development of combinatorial methods in electrochemistry, characterizing electrified interfaces by vibrational spectroscopy, in-situ surface diffraction studies and scanning probe techniques (including the Scanning Kelvinprobe), combining electrochemistry and surface science and describing electrified interfaces also with *ab initio* theoretical models. All groups in the department have their strong and independent research agenda but cooperate strongly on major questions and topics (see below).

Electrochemical reactions are of considerable scientific interest. Nearly all electrochemical reactions of practical importance are catalytic in nature. This is in particular true for elementary reactions like the hydrogen-evolution, the oxygen-reduction or the metal dissolution. Due to a lack of in-situ surface sensitive experimental techniques and due to a lack of theoretical modelling electrified interfaces, the depth of understanding is way behind the understanding of heterogeneous catalytic reactions in the gas-phase (see the recent Nobel Prize to Gerhard Ertl). Progress therefore only seems possible if suitable techniques and suitable theories are developed – this therefore is the major scientific focus of the department.

Besides scientific interest electrochemical processes are also of ultimate practical importance. The stability of engineering materials is determined by electrochemical reactions like the metal and alloy dissolution or the electroreduction of oxygen (corrosion and corrosion protection), energy storage

Fig. 1: *Laboratories of the Department of Interface Chemistry and Surface Engineering.*

(batteries) and energy conversion (fuel cells) are dominated by similar reactions like oxygen reduction or metal-dissolution and deposition (metal air-batteries) and electrogalvanising is in general based on electrodeposition reactions like the deposition of Zn and Zn-alloys.

The department is therefore in a unique position to combine quite diverse areas of industrial interest by their common underlying electrochemical re-actions. In order to further promote the field of electrochemistry the department together with the Ruhr Universität Bochum has founded a Center for Electrochemical Sciences. This Center combines the electrochemical expertise of both institutions and adds to this up to four Junior Research Groups in complementary fields of electrochemistry. The Center is funded as well by the State of North Rhine-Westphalia as by industry (TKS).

Electrochemistry is always linked to the chemical and electronic nature of the electrode under investigation. The Department therefore has a strong interest to combine the properties of the

solid state with the properties of the interface and the kinetics of the electron transfer reaction with the clear aim to optimize the stability of the material or its electrocatalytic properties. This is of particular importance for the steel based research activities of the department. As one example: the development of intelligent self healing coatings requires knowledge on the structure and storage of inhibiting molecules, knowledge of the electrochemically triggered release of these molecules and the interaction of the inhibitors with the corrosion surface leading to a reduction of the electron-transfer and ion-transfer reactions. This complex interplay is actually being studied in close collaboration with the MPI for Polymer Research and Fraunhofer in a large program financed by the Max Planck Society.

In the following, areas of central interest for the Department are summarized followed by a brief description of the major research interests of the Department's scientific groups.

Areas of Interest

Fundamental research in electrochemistry

Despite the existence of old mean-field theories for the description of the *ion distribution near interfaces*, there is still a lack of understanding especially for the regions were the mean-field description is breaking down. Experimentally, we are currently working on an evaluation of the ion distribution around surfaces under controlled potential using mainly ellipsometry. Of special interest are low ionic strengths in the electrolyte, where purely electrochemical experiments are hard to carry out.

Scanning electrochemical potential microscopy (SECPM) is a new technique to directly probe the potential distribution and structure in the diffuse double layer at an electrode interface. The initial experimental results were not understood and numerical FEM simulations were used to develop a basic understanding of the interaction of the double layers at the electrode and probe. Furthermore, the optimum shape of the probe and experimental conditions minimizing the perturbation of the electric double layer by the probe were studied (see highlight on p. 137).

The *oxygen reduction reaction* (ORR) is a fundamental electrochemical process of high importance in corrosion and fuel cells. Nevertheless, the mechanism is controversial and seems to strongly vary with electrode surface, pH and electrode poten-

tial. Several projects of the Department are dedicated to the ORR in a combined interdisciplinary research effort.

The structure including aqueous solvation and thermodynamic stability of a comprehensive set of possible intermediates of the ORR, generated from oxygen (O_2) by sequential addition of up to four electrons and protons have been studied with electronic structure methods developing two complementary approaches. A cluster approach combining an explicit first solvation shell with a polarizable continuum scheme allows an efficient and semi-quantitative evaluation of the chemical potential $\mu(\Phi,pH)$ of the intermediates as function of electrode potential and pH. On the other hand, molecular dynamics simulations with periodic boundary conditions allow a detailed study of the structure and dynamics of the solvation shell of the intermediates in bulk solution.

In spectroelectrochemical experiments on semiconductor surfaces we are currently searching for characteristic vibrational modes of the respective intermediates of the ORR using attenuated total internal reflection infrared spectroscopy. The first suggested intermediate is always the superoxide anion. To validate the computed vibrational frequencies and to study the chemical rather than electrochemical decomposition of solid KO_2, Raman and infrared spectroscopic experiments at different atmospheres, with variable humidity, are being carried out.

Two experimentally and theoretically well characterized surfaces have been selected to study the electrocatalytic and/or inhibiting effects of electrode surfaces. Gold has a high reactivity for ORR. The Gold(111)/water interface structure as function of pH and surface polarization is studied with *ab initio* DFT and will be used to investigate the catalytic effect on the ORR. On the other hand, zinc corrosion products including zinc oxide inhibit the ORR and the previously well characterized ZnO(0001) surface [1] will be used to study the effect of the ZnO/water interface on the ORR intermediates.
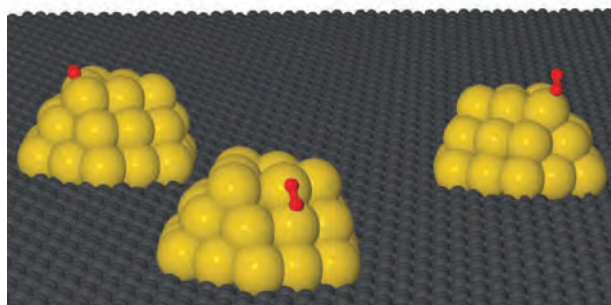
Fig. 2: *Catalysis of the oxygen reduction reaction on nanoparticles.*

Corrosion

For many materials their performance is critically determined by **corrosion on the micro- and submicro scale**. For instance, corrosion of aluminium alloys is governed by intermetallic particles in the size range from a few micro metres down to a few nano metres; also for novel zinc alloy coatings on steel the micro-structure of the different phases is assumed to play a crucial role for their performance. It is the aim of a current joint DFG research project together with the group of Prof. Schuhmann at RUB to develop new powerful investigation tools for studying the underlying mechanisms. In addition also the potential of SECPM is being investigated [2,3], as well as STM [4].

Metallic glasses, including Fe-rich materials called amorphous steels, lack crystallinity and, therefore, structural defects like grain boundaries or dislocations. For these reasons metallic glasses are sometimes considered superior in their corrosion behaviour in comparison with crystalline alloys. They are proposed for several applications from medical implant materials to special surface coatings. Nevertheless, the corrosion behaviour of such materials depends, like for all materials, very much on the specific environment and other conditions. One drawback is that upon aging or heat treatment a recrystallisation takes place with the consequence of creation of chemical inhomogeneity and structural defects. The final result is a regular nanocrystalline microctructure which is still homogeneous on a larger micrometer scale. With the study of corrosion behaviour of the amorphous steel $Fe_{50}CrMoBC$ we targeted the effect of heat treatment and induced microstructure changes on the corrosion behaviour in different solutions. The pristine amorphous steel shows a very high breakdown potential which is lowered considerably with the forming crystallinity (see p. 97).

While investigations on the delamination mechanisms of **Zn-Mg alloys** have led to quite good understanding [5], activities on the corrosion performance of Zn [6], Zn-Mg and Zn-Mg-X have been intensified, with emphasis on fundamental aspects of the corrosion performance of the multi-phased zinc alloys themselves and the role of corrosion product layers forming on the steel surface exposed on defects or cut-edges. For these investigations, artificial corrosion product layers are formed under different conditions and their properties are investigated, as well as the corrosion behaviour of model alloys prepared from the melt and electro-deposited single phase solid solution alloys [7].

Selective dissolution or dealloying is a detrimental corrosion process that is for example involved in stress corrosion cracking of stainless steels. At the same time, this process can be employed technically to produce a porous metallic material with nanometer scale ligaments (nanoporous metals). Such materials are used as catalysts. Noble metal binary alloys are both, the starting point for producing nanoporous materials and a simple model system for fundamental studies on dealloying as a corrosion process. Using a unique mix of modern characterisation techniques, e.g. employing synchrotron light, the single-crystal Cu_3Au system has been examined mainly focusing on the initial subcritical stages, including the influence of corrosion enhancers like Halides, as well as of model inhibitors. The peculiar surface structure developing on $Cu_3Au(111)$ has also been addressed in a collaboration to perform atomistic simulations (see p. 139).

In dry ambient atmosphere, corrosion rates of metallic alloys are extremely low. The corrosion attack gets much more severe either in contact with humidity or (reactive) liquids, or at elevated temperatures. In steam turbines the combination of both, humidity and high temperatures, leads to severe ***high-temperature corrosion***. In an in-house project the corrosion behaviour of binary and multicomponent Fe-Al alloys in steam at around 700°C is examined. While the binary versions with Al contents higher than 18% show low corrosion rates, the addition of third or even more elements leads in most cases to a deterioration of the corrosion resistance. These additional elements are necessary to achieve the target mechanical properties. For alumina formers it has been shown in oxidation experiments that the application of thin third element films on the surface can influence the stability of the material considerably. The film induces a direct growth of the stable alpha-alumina, while in the usual case first metastable alumina layers form and only later transform to the stable phase, but with a less perfect morphology. The initial scale growth in gas reactions at high temperature is a further focus. Here currently oxidation and sulphidation processes are studied.

Enhanced corrosion is also observed under very different circumstances, for example in the ***microbiologically influenced corrosion*** by bacteria like the marine sulfate reducing bacteria (SRB). Basic electrochemical experiments have been carried out using cultures of novel SRB strains with an outstanding corrosion activity in comparison to other well investigated strains [8]. Our general chemistry laboratory has now been extended with the necessary equipment (e.g. an autoclave and a thermostatic chamber) for sterile handling and incubation of anaerobic microorganisms at our department. The aim of this cooperation project with the Max-Planck-Institute for Marine Microbiology in Bremen is to improve the understanding of the fundamental electron transfer mechanism, by a combination of electrochemical techniques with surface analytics of corroded iron samples and corrosion product analysis.

Coatings and adhesion

Adhesion promotors in industrial applications are often organosilanes. While model systems usually consist of alkylsilanes, adhesion promotion happens through silanes with a second, different functionality, which can react with the material to which it should promote adhesion. We have studied the layer formation properties of two different silanes, Octyltrimethoxysilane and 1-Octenyltrimethoxysilane. Though chemically similar, their abilities to form ordered layers on oxide-covered silicon substrates are substantially different [9].

Although the investigation of the fundamental mechanism of corrosion driven **delamination of organic coatings** has been a topic of thorough investigations since quite a long time, still many open questions do exist. For instance, it is still disputed whether localised interfacial galvanic elements may play a role in the seemingly erratic path a filament in Filiform corrosion takes (see Fig. 3) or how the processes at the very frontier of cathodic delamination really look like. A better understanding of ion mobility along the polymer/metal interface is of crucial importance for this. With this aim a novel approach for studying migration along interfaces is applied [10].

Further work on polymer coated systems is directed towards obtaining an atomistic understanding of the structure and corrosion of the polymer-coated metal or oxide surfaces as a guide for future material design. With this aim, a multiscale simulation approach is developed to combine quantum mechanical DFT calculations, fully atomistic molecular dynamics, and coarse-grained molecular simulation. The first object of our research is the polyurethane/ZnO interface. At present the empirical OPLS-AA force-field is modified comparing DFT and classical calculations to reproduce adsorption of water and small polar organic fragments on ZnO(0001)-Zn-O/OH [1]. Predicted adsorbed states are stabilized by hydrogen and dative bonds. Their structure and stability agree well to previous theoretical results and experiments.

Water at interfaces is believed to play a crucial role in atmospheric corrosion, as well as in the delamination of coatings. Water as a liquid with a strong hydrogen-bonded network is, however, expected to have properties different from the properties of bulk water. An understanding of the binding situation is therefore crucial. Using infrared spectroscopic ellipsometry, studies are under way to characterize the **network structures of water films on solid surfaces**, as well as the difference of water at an air/water interface to the bulk water.

Surface morphology and in particular surface roughness and local chemistry significantly affect the physical and mechanical properties as well as fundamental interaction forces at surfaces and interfaces and play a critical role in advancing the performance of materials systems. However, no experimental study has been reported, that comprehensively describes the **interactions between rough surfaces in electrolyte solutions**. One reason for this are inherent limitations of most available experimental systems that make it difficult to control and vary critical system parameters in-situ while simultaneously performing interaction force measurements. We have designed an improved electrochemical AFM cell [11] which enables us to study adhesive interactions locally. Also, in cooperation with the University of California, Santa Barbara (Chemical Engineering Department, Prof. J.N. Israelachvili) an electrochemical surface force apparatus (EC-SFA) has been developed which is particularly suited for studying the interplay between surface roughness, confined interfacial fluid films and fundamental interaction forces. Using the newly developed experimental systems surface force measurements under electrochemical potential control reveal how increasing levels of surface roughness and dissimilarity between the potentials of the interacting surfaces influence the strength
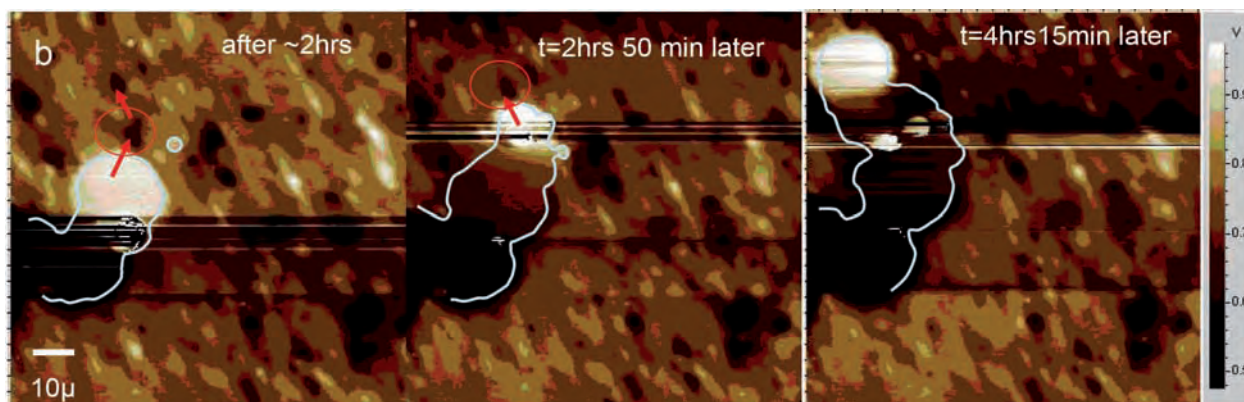

Fig. 3: *Series of surface potential maps showing the propagation of Filiform corrosion on a plasma polymer coated aluminium alloy. Light colours indicate anodic sites, dark colours cathodic sites. Note the cathodic intermetallic particles near the filament head.*

and range of electric double layer, van der Waals, hydration, and steric forces. [12].

Zinc coatings on steel are widespread in use for corrosion protection. New steels in use in automotive applications frequently cause problems due to segregation of certain alloying elements to the surface and a change in adhesion of coated Zn layers. Such processes are being studied at the institute for a long time. In modern coatings there are, in addition to Zn, often other elements required to obtain a better behaviour. Mg is one example, also Al which forms an Fe-Al interphase for better adhesion. Recently the Interface Structures group headed by Dr. Renner and the Molecular Structures group headed by Dr. Rohwerder performed in-situ X-ray diffraction measurements to follow the initial Zn *deposition from ionic liquids* on single-crystal model systems Au and Fe. In both cases a clear epitaxial relation was observed with a first growth of a pure Zn layer and the subsequent formation of alloy phases at the interface. Zn on Fe(111) for example grows in two domains rotated around the basal plane and developing four Fe-Zn domains at the interface with distinctive values for the rotation angles in between the substrate and the first Zn layer.

Functional surfaces and interfaces

The development of *coatings for intelligent corrosion protection* within the department focuses mainly on the application of conducting polymers. The understanding on how such coatings based on conducting polymers could work was further advanced [13,14], however some problems are still remaining. Especially for zinc as substrate it was found that an insulating interface seems to form inevitably between intrinsically conducting polymer (ICP) and metal, preventing corrosion triggered reduction of the ICP and thus release of corrosion inhibitors [15]. A first approach for solving this problem was tested and might prove to work reliably (see Fig. 4) [16].

Self-assembled monolayers have proven to be a useful model system for studying degradation reactions caused by intermediates formed during oxygen reduction at defect sites in these layers, thus simulating processes occurring during corrosion driven delamination. In the reporting period, a set of pyridinethiols and -disulfides was used for the investigations (in cooperation with Prof. Wöll (KIT)). A good correlation was found between ORR inhibition and film quality as a function of molecular chain length and immersion time in the SAM solution. The ORR could be shown to occur solely at defect sites, mainly at the domain boundaries. The results indicate that the currents generated at these sites are due to the one-electron reduction of oxygen to superoxide (O_2^-). The further reduction of (O_2^-) seems to be inhibited and also the desorption into the electrolyte seems
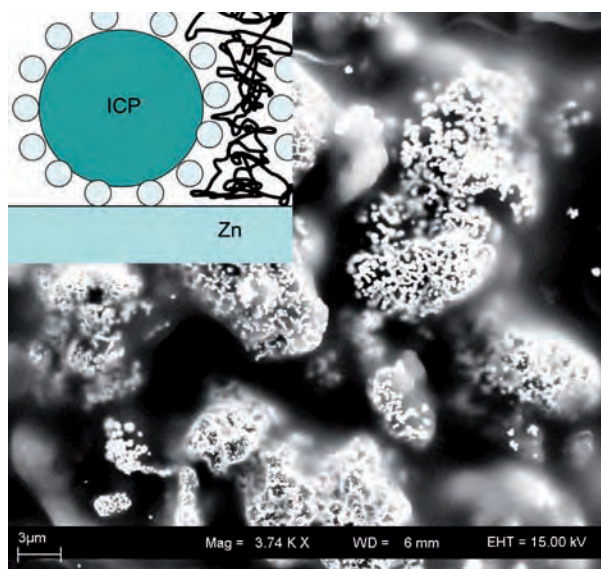

Fig. 4: *Top left: strategy for preventing the formation of unwanted insulating layer between conducting polymer and zinc. Electronically conducting nano particles serve as spacer. Main: SEM image of bottom side of a PANI containing clear coat stripped of the zinc surface: clearly visible are the (white) gold nano particles covering the larger PANI particles [16].*

to be significantly blocked, thus effectively inhibiting further ORR on these surfaces [17].

DFT studies of alkanethiol SAMs on Gold(111) have shown energetically favorable reconstructions by 1/6 monolayer of gold adatoms resulting in thiol-Au-thiol moieties. This leads to a stabilization mechanism that explains the hitherto unclear vacancy island (pit) formation experimentally observed in all SAMs on Gold. While initially the adatoms are taken from single-atom surface vacancies inside the SAM, this structure can further stabilize by vacancy diffusion to the domain boundaries [18,19]. The controversial van-der-Waals interaction between the alkane chains was also studied using correlated methods [20].

Among *metal nanoparticle catalysts*, Pt-nano-particles are currently the most potent catalysts for the ORR in PEM fuel-cell technology. In order to support and guide experimental work on the ORR on Pt-nanoparticles, a computational study is currently being carried out using quantum chemical methods that allow to treat charged systems and explicit as well as implicit treatment of solvent. This way, information can be obtained about the energetics of the reaction under different conditions, structural features and size effects. One interesting feature is the degree of surface oxidation of Pt nanoparticles. The results will aid in the search for better catalysts, like core-shell particles or alloy nanoparticles.

Improvements of the activity and stability of novel electrocatalysts like nanoparticles need to be achieved in order for them to become feasible

THE DEPARTMENTS

for future application in electrochemical energy conversion. We are studying the influence of the carbon support material on noble metal particles by systematically introducing surface functional groups with defined concentrations. The acquired knowledge shall be used to develop a "support-tuning" strategy and an attempt to design high performance oxygen reduction catalysts with increased lifetime.

A novel approach for investigating the degradation of metal nanoparticles due to electrochemical treatments has been developed [21,22]. Identical-Locations of materials can be located repeatedly in a Transmission Electron Microscope (IL-TEM), therefore enabling a direct comparison of alterations in the structure of for instance Pt fuel cell catalysts over time. In future this will be extended to alloy particles and the investigation of surface segregation [23] utilizing the high-resolution TEM in cooperation with Dr. A. Kostka.

With the German Federal Government's Economic Stimulus Package II of 2009 (see p. 31), the Department participates in Government-sponsored activities to prepare for the future age of electromobility. Electrochemistry and *batteries* are, among many other technical issues, in the core of the projects related to the German economic stimulus program. Within this project the group of Dr. Rohwerder will evaluate the feasibility of scanning Kelvin probe measurements for following the lateral diffusion of Li ions. Dr. Renner and his group focus on in-situ X-ray diffraction using synchrotron radiation and in-house methods like scanning Auger microscopy or atom probe tomography. All studies will be based on thin films and other model systems. A new pulsed laser deposition setup will allow here for the deposition of anode, solid-electrolyte, and cathode materials.

Al doped ZnO surfaces are important components of thin film solar cells, where they not only serve as transparent electrical contacts but also increase the efficiency by introducing a light scattering effect at the interface. Utilizing an *electrochemical etching* approach we are able to systematically alter the surface morphology by selective leaching of highly active sites like grain boundaries, which is in contrast to the generally used uniform chemical etch that is only dependent on diffusion. In cooperation with the FZ Jülich we try to understand the relation between these ZnO surface structures and the solar cell performance, and will continue to optimize the texturing procedure by varying the process parameters in a high-throughput approach.

Processes

As part of the activities in the Christian Doppler Lab for Diffusion and Segregation during Production of High Strength Steel Sheet a novel approach for detecting hydrogen in steels is being developed, based on the Kelvin probe technique (see p. 117).

Grain boundary oxidation during hot rolling can be a considerable problem in the following processing steps, such as selective etching during pickling. In the Christian Doppler Laboratory for Diffusion and Segregation it is tried to assess the origin of enhanced grain boundary oxidation and to simulate the built up of the grain boundary oxides (see p. 64).

The fundamental investigation of *hot dip galvanizing* has been the successful object of a consecutive number of RFCS projects, where the main focus has been in the recent years on optimizing the annealing atmosphere in order to suppress external oxidation. However, still some activity was devoted on the investigation of the galvanizing process itself. It was found that not only the extent of external oxidation plays an important role but also the morphology, i.e. especially the typical length scale of the oxide islands. Furthermore, the length scale of the oxide islands seems to scale with the overall coverage for a given alloying element [24]. Many commercial steels show a quite nano-structured morphology leading to comparatively high wetting kinetics compared to binary model alloys such as Fe-Si or especially Fe-Mn, which show much slower wetting at the same oxide coverage. Aim of future activities will be to study the possible reduction of external surface oxides by alloying elements in zinc alloy melts.

In a collaboration with a Japanese steel manufacturer, the Zn *wetting behaviour* on oxide layers with a defined pattern applied on steel surfaces has been addressed to evaluate the influence of pattern length scales. At length scales down to a micrometer the wetting behaviour scales linearly with the oxide coverage. The equipment was upgraded to perform studies with the higher-melting Al; also experiments to examine Al welding processes thus became possible.

Closely related to the activities on hot dip galvanizing are the activities on *selective oxidation and segregation during recrystallisation annealing*. Within the RFCS project Novanneal it was found that lowering the hydrogen level and increasing the dew point has considerable potential in improving galvanizing of many steel grades, but are not sufficient for all cases, such as for many TRIP steels. Hence, current activities focus on the potential of an iron oxide top layer as barrier preventing selective external oxidation of alloying elements, either by application of a layer of iron oxide nano-particles that are reduced during annealing (RFCS project Ferrigal), which works for galvanizing but so far causes adhesion problems, or by forming an oxide layer during the initial phase of annealing to be kept at a constant thickness and which is then reduced during cooling (RFCS project HEAT). For the latter

strategy the kinetics of oxidation and reduction of the oxide layer need to be understood in depth. Detailed studies are carried out. Especially worth mentioning is the successful development of a quartz micro balance for in-situ investigation of high temperature oxidation processes.

The co-deposition of silica particles during electro-galvanising is a prerequisite for using encapsulated mesoporous silica particles as reservoirs for corrosion inhibitors to be deposited into the zinc coating. A concept for successful deposition could be devised and was successfully tested.

Though the *phosphating process* is used in industry in different variations for over 100 years, the nucleation of phosphate crystals is not well understood. Crystal nucleation in general is a topic under discussion at the moment. In a collaboration with Salzgitter Mannesmann Forschung GmbH, we are focusing on studies of the surface activation and an initial phase of crystal growth in the phosphating process. In this project, novel steels containing passive materials in its surface are investigated. In the near future, we hope to extend studies to novel conversion coatings which are under discussion to replace the current phosphating process.

Research Groups

Molecular Structure and Surface Modification (M. 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 of 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

In cooperation with Prof. Wöll (KIT) 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, also involving reactivity of heme proteins adsorbed on the SAMs [17] as well as reduction of adsorbed metal ions. Another important aspect is the mobility of ions along interfaces [10]. On a more applied scale the role of contaminations at polymer/metal interfaces are of importance [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. This enables application of the SECM exactly on the same features as mapped by SKP. Furthermore, work on SECPM (Scanning Electrochemical Potential Microscopy) is being carried out [2,3]. In addition, the direct application of the AFM based Kelvin probe technique (SKPFM) for the in-situ study of Filiform corrosion on aluminium alloys could for the first time provide direct proof for the role of the intermetallic particles for determining the direction of the filament pathway (see Fig. 3).

Tailoring of the surface oxide provides direct control of the stability at the polymer/metal interface and also to some extent of the corrosion behaviour in general, as was shown for zinc alloys [5], but also zinc itself and its oxides are still not fully understood [6]. Typically, such alloys are multi-phase systems making it difficult to study the corrosion behaviour of a certain oxide composition. Hence, pure phase systems are tried to be prepared electrochemically. So far only with slight success from ionic liquids [7], but recently a break-through was reached with deposition from THF. Another question which is investigated is the role of zinc corrosion product layers precipitating on exposed steel surfaces. These corrosion product layers are generally of hydroxide and oxide nature. Strong indications were found that the role of Mg in zinc alloy coatings for cut edge corrosion protection lies in changes in the corrosion product layers occurring already in the very initial stages of corrosion. Focus of current investigation is on the long term performance.

3. Wetting and interfacial reactions at metal/metal melt interfaces and selectice 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 [24]. The latter sensitively depends on the annealing conditions and the correlated selective oxidation prior to the hot dip galvanising which is another topic of research, as well as grain boundary oxidation during hot rolling (see p. 64).

4. Intelligent self-healing concepts for corrosion protection

Intelligent self-healing capabilities of organic and inorganic coatings are of central importance for the production concepts of the future. While we have now fully understood how an intelligent coating should look like for being able to provide intelligent corrosion protection [13,14], i.e. the release of inhibitors only in case of corrosion, still problems exist with either severe corrosion at the interface between the coating and the metal or with the formation of an insulating interface (especially on zinc) [15]. Strategies to overcome these problems involve decorating the particles of conducting polymer with electrically conducting nano particles [16].

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

In the reporting period the SKP technique was successfully adapted for in-situ use in synchrotron set-ups, where the effect of beam-induced surface resp. interface charging was investigated on different inorganic materials and biomembranes (see p. 119), as well as for spatially resolved high-sensitivity hydrogen detection (see p. 117).

Interface Spectroscopy (A. Erbe)

Currently, the interface spectroscopy group has two major working directions. The first direction is the design of surfaces for spectroscopic studies of interfaces with the main aim of characterising surfaces in complex environments, especially under electrochemical conditions. The second direction is a modification of material's interfaces by chemical means to change surface properties and to make surfaces durable and resistant to attacks from an environment.

The motivation for doing optical design of interfaces is the need for understanding surfaces in environments different from ultra-high vacuum conditions. Optical techniques are in principle a convenient tool to access interfaces also in liquids and polymers. Therefore, we use optical spectroscopy from the ultraviolet to far-infrared wavelength range for investigations of interfaces. Novel instrumentation which were established recently include a mid-infrared ellipsometer and a microscope for mid-infrared spectroscopic imaging.

Details of part of the project to design surfaces for fundamental studies can be found as a scientific highlight in this report. We succeeded in realising a system which, by introduction of a semiconductor interlayer between metal film and medium of incidence, shows an increased transmission of light through the metal films, and consequently increased absorbance of a sample in contact with the liquid medium [26,27].

Computations using the finite element method (FEM) to solve the Maxwell equations have been used to compute infrared absorbance spectra from rough surfaces [28]. So far, we have focused on understanding surface enhanced infrared absorption spectroscopy, and to compute full spectra obtained from non-planar surfaces. In the future, we would like to generalise the technique employed to make further optical methods useful for analysis of rough surfaces as encountered in "real" materials. A further aspect of this kind of research is the understanding of the look of a surface, as perceived by eye.

While good analytics is needed in order to understand surfaces, we do furthermore intend to use the insight gathered from proper surface analysis to modify interfaces, and to study the modification of interfaces under the influence of the ambient environment. Some of the related-projects have been discussed at the beginning of this section.
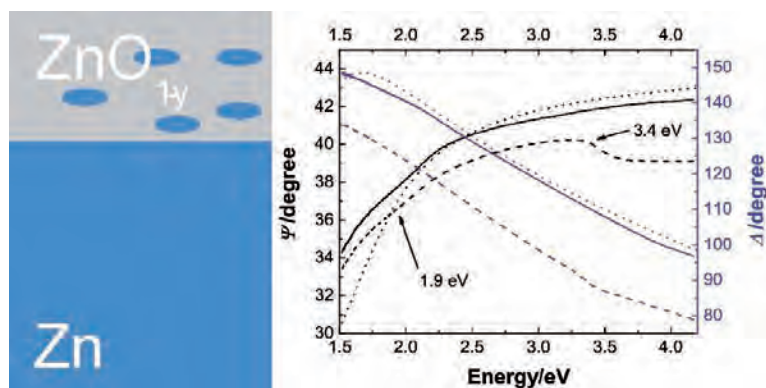

Fig. 5: *Ellipsometric spectra of the native oxide film on zinc show a typical absorption of zinc-doped zinc oxide around 1.9 eV. After electrochemical reduction, the absorption corresponding to the oxide band gap at 3.4 eV disappears [29].*

Chemical transformations at an interface could be characterised in a study of the native oxide film on polycrystalline zinc. The main finding here, analysing the Auger peaks in the X-ray photoelectron spectra and spectroscopic ellipsometry data (Fig. 5), is that the film is strongly doped with metallic zinc, therefore behaving substantially different from bulk zinc oxide [29]. Current investigations using spectroscopic ellipsometry and electrochemistry aim at finding changes in electronic structure of the native oxide films during exposure to air, humidified air, and humidified argon atmosphere.

In addition, we provide support to the whole institute in application of optical characterisation techniques. An important example is the optical characterisation of biological photonic structures in collaboration with the Department of Microstructure Physics and Metal Forming, as discussed as scientific highlight elsewhere in this report.

Fig. 6: *Simulation of the twin polymerization process – from molecular precursor (left – structure and electrostatic potential), to oligomer, to nanostructured hybrid polymer (right – result of coarse grained simulation and actual material monolith).*

Atomistic Modelling (A. Auer)

Work in the atomistic modelling group is focused on the application of electronic structure theory and simplified models for the investigation of molecular and supramolecular systems in spectroscopy, electrochemistry and material science. With a focus that is complementary to the scope of the CM department, the expertise of our group is a valuable addition to the spectrum of simulation techniques at the MPIE.

Besides method development and application of highly accurate methods to smaller molecular systems (see group profile of the new Atomistic Modelling group, p. 15) the main interest of our group lies in the description of key processes in electrochemistry using a broad variety of methods ranging from electronic structure approaches to FEM techniques (see p. 27, p. 54, p. 137). The Atomistic Modelling group is dedicated to a close interaction with the other groups of the department in the areas of electrochemistry and surface spectroscopy (see p. 54).

Another area of interest is the field of material science, where two projects aim at a deeper understanding of the interplay between soft and hard matter and interfacial structures.

In collaboration with Prof. N. van der Vegt (TU Darmstadt) and ICAMS (see p. 28) a multi-scale simulation of the polyurethane/ZnO interphase is being developed (see p. 56).

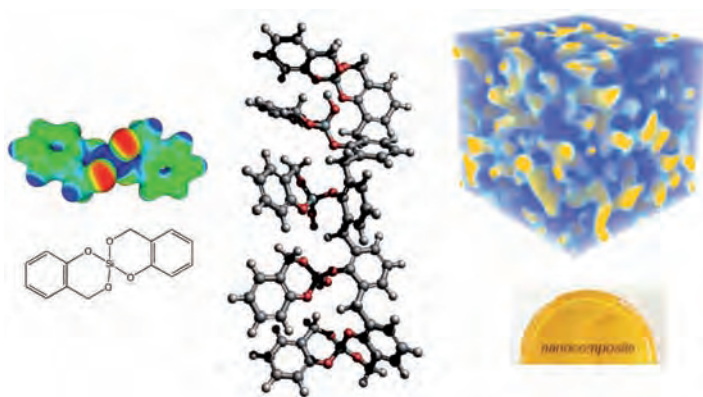In the framework of a collaboration with the TU Chemnitz a novel type of polymerisation is investigated that offers the possibility to synthesize organic/inorganic nanocomposites with structures of the size of a few nm from a single monomer [30]. Theoretical studies on structure and energetics of the most important reaction steps and possible side reactions have been carried out. In order to simulate structure formation at the nm lengthscale, a multi scale modelling approach is currently being devised (see Fig. 6). In this technique results from DFT calculations [31] are used to parametrize a combined dissipative particle dynamics / kinetic monte carlo simulation to describe the diffusion/segregation and network formation processes.

Electrocatalysis (K. Mayrhofer)

The newly established electrocatalysis group at the department will focus on the activity, stability and selectivity of electrode materials for heterogeneous reactions. In order to gain a fundamental understanding of various electrochemical processes at the solid-liquid interface, all three of these sub-domains are approached concertedly. This is achieved by a versatile combination of complementary characterization techniques, investigation and comparison of the behaviour of well-defined and real material surfaces, and numerical simulations.

Scientifically the interests of the group include the essential oxygen reduction reaction, locally-resolved electrochemistry in particular related to corrosion phenomena, as well as electrochemical energy conversion. The technological focus is placed on the development of in-situ electrochemical investigation techniques that simultaneously provide information on reaction kinetics, reaction products, and electrode surface state and composition. Furthermore, there is a continuous interest in the transfer of the fundamental know-how on corrosion and electrochemical energy conversion to industrial applications.

Electrochemistry and Corrosion (A.W. Hassel)

Research of the Electrochemistry and Corrosion group continued in electrochemical materials science with an emphasis on microstructure, crystallography and reactivity to allow for a thorough understanding of the reaction mechanism and their use for process design on a nanoscopic and even atomic level. Research areas addressed were:

i. metallic nanowires and nanodevices

ii. corrosion and new techniques

iii. design of passive films and nanostructured surface films

iv. combinatorial alloy development and high throughput experimentation

i. the methodological combination of directional solidification and subsequent electrochemical processing has been extended to other systems and was used to create single crystalline nanowire arrays from W [32,33], Mo [34,35], Si [36] and Au [37] or even alloys [38]. Various properties were studied including the anisotropic mechanical properties of nanowires [39] and in particular the chemical properties of uncommon crystallographic surfaces such as the 110 surface of Au nanobelts and plates [40,41]. This project was part of the priority research area of the DFG and an overview over the achievements has been summarized in a concluding review [42].

ii. surface reactions were studied e.g. on NiTi to explore new strategies for its surface engineering by nitridation or selective oxidation [43,44]. Following the tradition of the electrochemistry and corrosion group novel experimental set-ups have been developed including an impedance titrator [6], an electrochemical in-situ tensile tester [45] and an extension of the scanning droplet cell with electrolyte analytics [46]. The latter has been applied to study electrochemical texturing of ZnO films [47].

iii. based on the expertise in passive films further research was directed towards the formation of oxide/oxide structures [48] passive films with embedded Au nanoparticles [49] or subsequently implanted oxide films [50]. Precise control over the passive film under electropolishing conditions of NiTi [51] a quantitative optical recognition of passive film thickness [52] and the grain dependent properties of polycrystalline β-NbTi alloys were also subject of interest [53,54].

iv. a very successful approach to materials science is the combinatorial approach in which composition spreads are studied by scanning microelectrochemical techniques. Various valve metal libraries have been studied combining metals that form insulating or semi-conducting oxides and those in which the parent metals are fully miscible or presenting a miscibility gap. Comprehensive characterisations were performed in the systems Hf-Ti [55], Ta-Ti [56], Nb-Ti [57], Hf-Ta [58] concerning the properties of the resulting passive films. In an attempt to further develop this approach not only theoretical considerations concerning the film formation were made [59] but also new systems relevant in corrosion science were studied such as the Al-Cu system [60]. Further experimental developments are presently combining scanning electrochemical investigations with downstream analytics of the electrolyte to quantitatively identify reaction products [46].

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

The group „Interface Structures and High-Temperature Reactions" focuses on nanometer and atomic-scale structural studies of surfaces in contact with corrosive gas atmospheres at high temperatures and electrolytes. A special emphasis is placed on in-situ X-ray diffraction techniques using Synchrotron radiation. Synchrotron light developed in the last
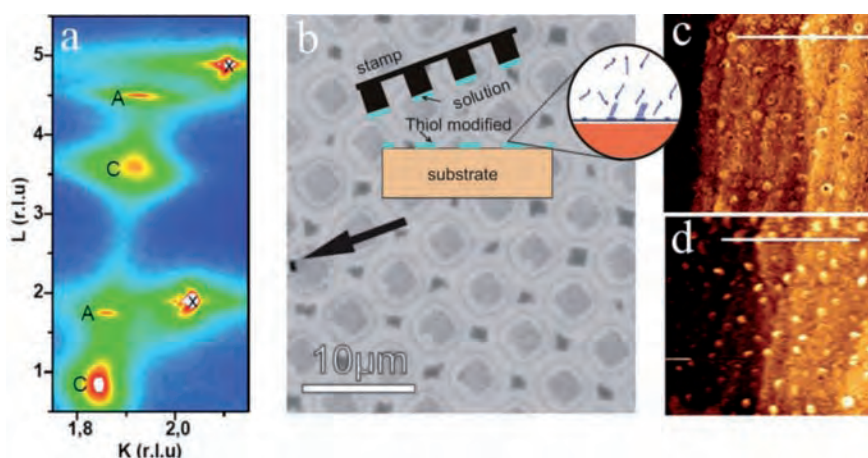

Fig. 7: *Dealloying: Reciprocal space map of a thiol-modified Cu_3Au system at 650 mV (a) and localized dissolution caused by thiol μcp (b). The corroding area by in-situ AFM at rising potentials (c,d, 450 nm scale).*

decades to be an important tool for materials science. Its capability to resolve atomic-scale structures even of low-dimensional objects is very beneficial for corrosion science. Also the possibility of *in-situ* experiments is an advantage.

Metallic model systems and in particular single crystal surfaces and epitaxial (textured) thin films provide a means to elucidate detailed mechanisms from various processes from oxide scale formation to Li-ion battery interfaces. One topic is how surface modifications and the application of thin oxide films influence and control the further oxide scale growth at high temperatures. Similarly, to give one more example, surface modifications like thiol layers are studied as model inhibition processes in aqueous electrolytes. Fig. 7 shows the example of the influence of an applied Thiol layer on the dissolution of Cu-Au. The onset of dissolution is shifted to larger potentials and the initially formed passive Au film is considerably stabilised. Only at very high potentials a Au peak close to the substrate peak is observed (A, X, Fig. 7a) while the initially formed twin Au peak (C, Fig. 7a) is still stable. This finding has been employed to produce a localised corrosion attack by applying a Thiol film pattern by µ-contact printing (in collaboration with Dr. Asif Bashir) and the initial stages were studied with in-situ atomic force microscopy (AFM, in collaboration with Dr. Markus Valtiner, Fig. 7c,d). New insights in the way inhibition works at the atomic scale could be obtained.

Next to dealloying, corrosion of metallic glasses, electrodeposition from ionic liquids, or battery processes, also high temperature corrosion is studied in various atmospheres. Fig. 8 shows e.g. the oxide scale on FeAlTi formed at 650°C in steam. These works will be continued using more high-resolution methods and in-situ diffraction to study the initial stages of this and similar processes in the future.

Christian Doppler Laboratory for Polymer/Metal Interfaces (G. Grundmeier)

The CDL for Polymer/Metal Interfaces funded by the Christian Doppler Society in Austria was established at the MPI für Eisenforschung in April 2003 and cooperates with voestalpine Stahl Linz and Henkel Austria as industrial partners. Although Prof. Grundmeier took over the position of a full professor at the University of Paderborn, the laboratory was proceeded at the MPIE in Düsseldorf to guarantee the continuation of the work until its end in December 2010. In the last two years three scientific co-workers worked in the frame of three research modules at the MPIE. Beside the module 4 which was established in 2007, a fifth module with Miba Gleitlager GmbH as new partner started in December 2008 at the University of Paderborn dealing with molecular adhesion promotion studies at polymer/copper alloy and polymer/aluminium alloy
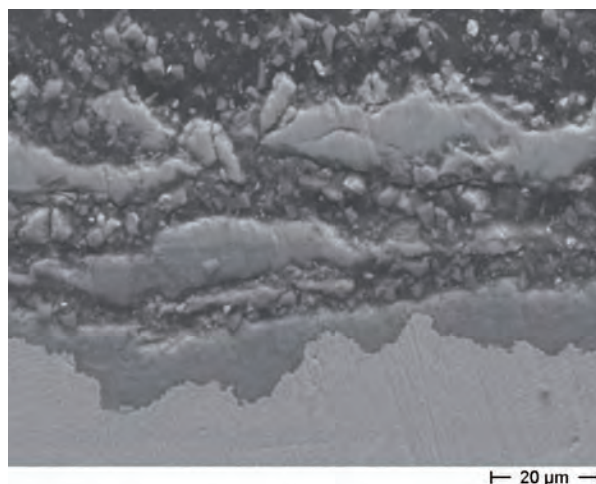

Fig. 8: *Cross section of FeAlTi after corrosion at 650°C in steam.*

interfaces. Within the CDL modules at the MPIE electrochemical set-ups were combined with other analytical tools like a miniature stretching apparatus (defect formation), an FTIR-ATR cell (water uptake and changes in interfacial composition) or the Raman apparatus (degradation of thin conversion layers during oxygen reduction reaction) to get in situ information of changes in the layered system during a corrosive exposure. Complementary investigations were dedicated to the molecular understanding of adhesion based on the application of Chemical Force Microscopy and Single Molecule Adhesion studies. These studies were combined with quantum mechanical simulations in cooperation with the department of Prof. Neugebauer.

Research module 1: "*Understanding of the electronic and adhesive properties of passive films on Zn alloy coatings*"

The measurement of interactions of single macro-molecules (poly(acrylic acid)) at the electrolyte/single-crystal interface of ZnO(0001) [61] and the correlation of topography dependent analysis in the pH range of stable ZnO with quantum mechanical simulations were very successful. Both experiments and theoretical calculations showed that carboxylic acid functionalities adsorb weakly to hydroxide-stabilised polar ZnO(0001)-Zn surfaces (molecular forces of 60-80pN) whereas they strongly bind to the separating step-edges between the polar terraces most probably via coordinative bonds (molecular forces of about 700 pN). This correlation is of high significance for further research in the field of adhesion promoters and adhesive development for galvanised steels.

Research module 2: "*Correlation of microstructure of the substrate and the layer formation as well as the formability of thin hybrid conversion coatings*"

The formation of microscopic defects of thin conversion coatings on galvanised steel substrates was studied using a miniature stretching apparatus.

A combination of this with an electrochemical three electrode set-up connected via a small capillary allowed the in situ analysis of the defect formation during forming of the substrate [62]. Complementary microscopic measurements by means of FE-SEM and EBSD in combination with Scanning Kelvin probe and SKPFM studies allowed the understanding of the forming behaviour of the conversion layers and its effect on corrosion protection of the substrate.

Research module 3: "Adhesion of polymer coatings on modified Zn alloy surfaces in environments of high water activity"

Fundamental investigations of cut edge corrosion behaviour at the polymer/zinc oxide/zinc interface were performed by means of the Height Regulated Scanning Kelvin Probe Blister-Test (HR-SKP-BT). First experiments showed that a blister solely grew by applying high electrolyte pressure (500 mbar) while the topography of the blister did not change significantly at low electrolyte pressure (100 mbar) [63]. Moisture reduction (97%→82%) resulted in a decrease of the cathodic de-adhesion kinetics by a factor of two to three. Further experiments with variation of the polarisation potential of the defect region to more negative potentials showed that the polarisation is more effective for the investigation of delamination progress than an increase of the hydrostatic pressure of the defect electrolyte [64].

Christian Doppler Laboratory for Diffusion and Segregation Mechanisms during Production of High-Strength Steel Sheet (M. 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 and developing a new simulation tool

for describing GB oxidation on a theoretical level. Although one might think that at grain boundaries there might always be an advancing front of internal oxidation, for none of the investigated binary alloys this was found to be the case. Exceptions are very low concentrations of e.g. Si or ternary alloys forming mixed oxides. This is object of intense current investigations. The simulation approach is based on an alternating cycle of calculating the element diffusion and chemical reaction. This new simulation tool called ASTRID (Applied Simulations of Thermodynamic Reactions and Interphase Diffusion) works by linking the thermodynamic database from ChemApp (GTT-Technologies, Germany) with the numerical programme COMSOL (COMSOL Inc., USA) and is able to simulate grain boundary oxidation (see Fig. 9). Good agreement with experimental results for the oxidation depths and the spatial phase distribution could be achieved e.g. in the case of iron-chromium alloys.
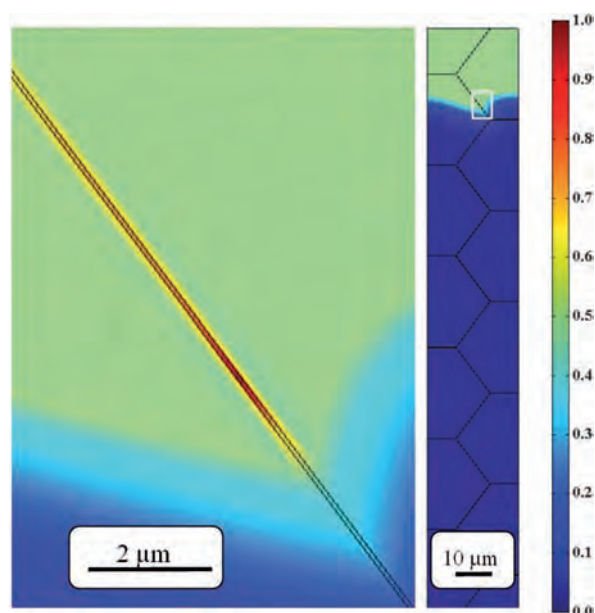

Fig. 9: *Spatial distribution of Cr_2O_3 and $FeCr_2O_4$ grain boundary (left) and oxidation depth (right) in Fe-3wt% Cr after oxidation at 650 °C. Relative intensity scale.*

P (Pickling) Module:

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

H (Hydrogen) 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. Here a main focus in the reporting period was on developing a novel method for spatially resolved highly sensitive hydrogen detection (see p. 117).

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Research Projects in Progress

Electrocatalysis

Meier, Mayrhofer: Metal-support interactions in electrocatalysis

Katsounaros, Meier, Mayrhofer: Particle size effect for the ORR

Topalov, Mayrhofer: ICP-MS for on-line elemental electrolyte analysis

Klemm, Mayrhofer: Microelectrochemical texturing of ZnO

Meier, Hodnik, Katsounaros, Mayrhofer: Stability of Pt und Pt-alloy nanoparticles

Electrochemistry and Corrosion

Diesing, Bruder, Hassel: Electronic tunneling in metal-insulator-metal contacts

Hassel: Combinatorial electrochemistry for the development of improved Ni based alloys

Klemm, Hassel: Combinatorial material development of ternary Al-Mg-Zn alloys

Mardare, Wieck, Hassel: High throughput screening of band gap engineered materials

Mardare, Wieck, Ludwig, Savan, Hassel: High throughput screening in combinatorial alloy development

Merzlikin, Mingers, Hassel: Hydrogen determination in coated steels

Merzlikin, Hassel: Hydrogen induced embrittlement of cold rolls

Milenkovic, Hassel: Gold nanostructures by directional solid state decomposition of Fe-Au alloys

Milenkovic, Hassel: Application of directionally solidified nanowire arrays

Neelakantan, Eggeler, Hassel: Microstructural aspects of passivity and corrosion of NiTi

Sanders, Hassel: Metal corrosion in contact with clay

Venzlaff, Widdel, Stratmann, Hassel: Microbiologically influenced corrosion of iron by sulfate reducing bacteria

Woldemedhin, Raabe, Hassel: Surface reactivity of β-Ti alloys

Atomistic Modelling

Biedermann : Gold/water interface - Structure as function of potential

Biedermann, Berezkin : ZnO/water interface - Structure as function of pH

Biedermann : Oxygen reduction - Intermediates in aqueous solution: solvation structure and energetics

Hamou : SECPM - charge and potential distribution at polarized electrodes, continuum simulations

Hamou, Erbe, Biedermann : Simulation of the structure of electric double layer/ ion distribution near interfaces

Berezkin : Polyuretan/ZnO Interphase structure and properties - network formation, adhesion, diffusion

Auer, Schneider, Benedikt : Theoretical studies on the ORR at Pt-Nanoparticles

Auer : Method development on highly accurate *ab-initio* electronic structure methods for large molecular systems

Auer, Benedikt (in cooperation with W. Hackbusch, MPI-MIS) : Tensor decomposition techniques in electronic structure methods

Auer, Berezkin (in cooperation with S. Spange, TU Chemnitz) : Theoretical studies on novel polymerisation techniques for nanoscale hybrid materials

Auer, Schneider (in cooperation with M. Mehring, TU Chemnitz) : Reactivity and structure of heavy main group element compounds

Auer : Benchmark studies for the quantitative prediction of NMR properties

Christian Doppler Laboratory for Diffusion and Segregation during Production of High Strength Steel Sheet

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

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

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

Swaminathan, Hüning: Segregation and oxidation of alloys

Swaminathan, Hüning, Borodin: Fundamental investigation of grain boundary oxidation

Molecular Structures and Surface Modification

Ankah, Rohwerder (in cooperation with F. Renner and G. Eggeler, RUB): Combined AFM, SEM and TEM investigation of the de-alloying behaviour of copper-gold intermetallic phases.

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

Borissov, Rohwerder: Ionic liquids for zinc alloy deposition

Borissov, Rohwerder (in cooperation with F. Renner): Interfacial reactions during electro-deposition from ionic liquids

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

Keil, Vogel, Rohwerder: Nano-particular iron oxide films for improved wettability

Keil, Bashir, Rohwerder: Characterization of zinc alloys for automotive application

Keil, Salgin, Vogel, Rohwerder: SKP as online analytical tool in synchrotron beam line

Khan, Rohwerder (in cooperation with F. Marlow, MPIK): Intelligent corrosion protection by nanocapsules incorporated to the zinc coating: understanding co-deposition

Krieg, Borissov, Rohwerder: Investigation of cathodic self-healing at cut-edge

Liu, Rohwerder: Fundamental investigation of hot dip galvanizing

Muglali, Rohwerder (in cooperation with C. Wöll, KIT): Oxygen reduction at self-assembled monolayer/gold interfaces

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

Sathirachinda, Salgin, Rohwerder: Electronic structure of native oxides in dependence on the atmosphere

Sathirachinda, Rohwerder: Application of SKP for the study of solid state and polymer electrolytes

Senöz, Rohwerder (in cooperation with W. Schuhmann, RUB): Combining SECM and SKPFM for the investigation of localised corrosion

Vimalanandan, Rohwerder: Intelligent corrosion protection coatings

Vogel, Schönberger, Rohwerder: QCM for high temperature application

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

Interface Spectroscopy

Reithmeier, Erbe: Infrared-transparent metal electrodes

Vasan, Erbe: Finite element simulation of surface-enhanced infrared absorption spectra

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

THE DEPARTMENTS

67

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

Murakami, Schneider, Renner, Erbe: Phosphating under electrochemical control

Ebbinghaus, Erbe: Distribution of sulfate and ammonium ions near semiconductor surfaces

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

Tecklenburg, Erbe: Surface tension of organosilanes in organic solvents

Chen, Erbe (cooperation with F. Hamou/U. Biedermann): Structure of the electrochemical double layer probed by ellipsometry

Chen, Schneider, Erbe: Kinetics of structural changes in the native oxide layer on zinc

Deb, Vasan, Ebbinghaus, Keil, Kostka, Erbe: Characterization and surface modification of iron oxide nanoparticles

N.N., Reithmeier, Erbe: Formation of self-assembled monolayers from solution

Marie-Curie-Outgoing Project

Valtiner (in cooperation with J. Israelachvili, UCSB): Novel concepts for molecular interface engineering and unravelling of structure/property relationships at electrified interfaces

Interface Structures and High Temperature Reactions

Ankah, Pareek, Rohwerder, Renner: AFM and in-situ diffraction studies on dealloying of Cu-Au alloys.

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

Bashir, Ankah, Valtiner, Renner: Thiol u-contact printing for inhibition studies

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

Duarte, Serrano, Romero, Stratmann, Renner: Corrosion of amorphous steels

Izzuddin, Renner: Sulphidation of Ni-Al alloys

Meimandi, Renner: Dealloying of Cu-Pd

Meimandi, Zabel, Renner: Initial oxidation of modified Fe-Al alloys

Naraparaju, Christ, Kostka, Renner: TEM investigation on shot peening effects

Pareek, Borissov, Rohwerder, Renner: In-situ diffraction studies on Zn electrodeposition from ionic liquids

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

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

Department of Microstructure Physics and Metal Forming

D. Raabe

Scientific Concepts

We conduct basic research on the **mechanical properties** [1] of materials and their relationship to the underlying **nano- and microstructures**, Fig. 1. The focus lies on **engineering materials** such as steels, titanium, magnesium, nickel, copper, intermetallics as well as biological and metal-based composites. These materials are characterized by complex phase and defect substructures. Consequently, our approach is based on using **advanced characterization** methods from the single atom level up to the macroscopic scale (e.g. tomographic atom probe [2,3], 3D EBSD [4-8]), **mechanical experiments** under well-controlled boundary conditions (e.g. joint in-situ strain and temperature mapping, micro-beam bending, indentation) [7-15], and **models** of microstructure evolution and microstructure-property relations at different length scales (e.g. *ab-initio*-based **multiscale** models in cooperation with the department of Prof. Neugebauer) [16-25]. Close interfacing of **simulation and experiment** with the aim of **quantitative** comparisons between the two has high priority in our concept [1,25]. As the microstructure of engineering materials evolves under complex thermomechanical history and boundary conditions, the effect of **processing** on the microstructure evolution and hence on the final mechanical response of the materials is taken into consideration (e.g. ultra-fine grained dual phase steel design through thermomechanical processing) [26-42].

The most important strategic scientific developments in the department in the past 2 years were the opening of a new group on **Atom Probe Tomography** (APT) in 2010 (p. 16, 21) [2,3], the increasingly close cooperation with the department of Prof. Neugebauer in the field of **multiscale modeling** [16,18-21], and the strengthening of our activities in the field of mechanism-oriented **alloy design** (p. 105) [2,16,19,20,38].
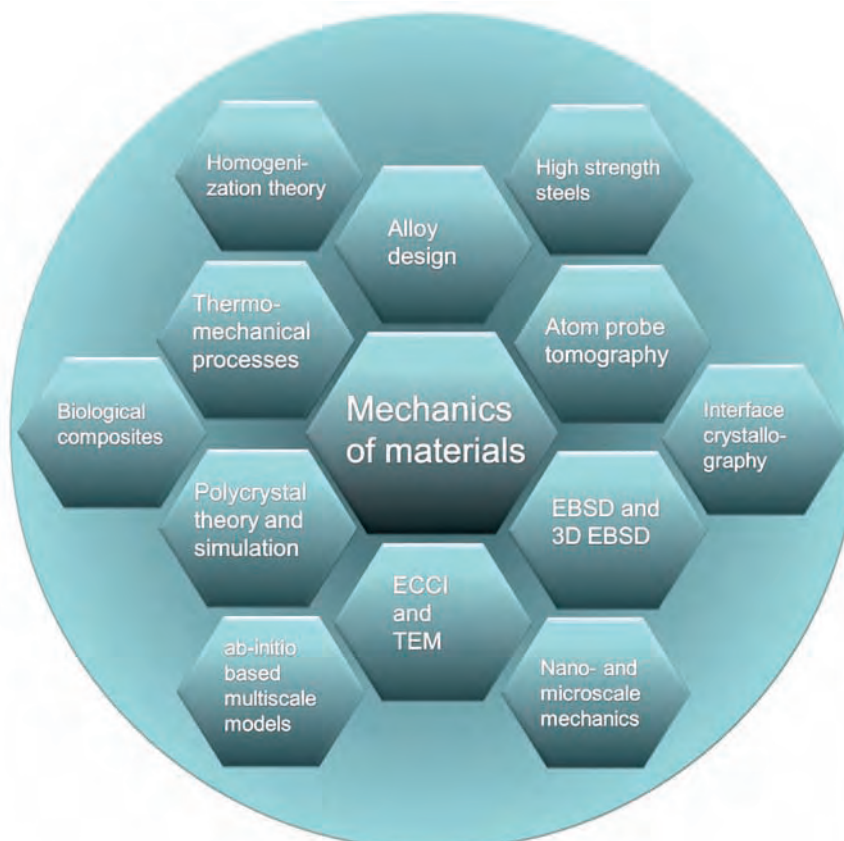
Fig. 1: *Main research areas in the department.*

Examples of recent projects involving atom probe tomography are the analysis of Mn partition effects in TWIP and TRIP steels (p. 105) [2], interface segregation in superalloys, and the composition of nano-precipitates in soft magnetic steels (p. 103).

Important projects demonstrating the strong inter-departmental links in the field of multiscale modelling are the *ab initio* prediction and subsequent constitutive use of stacking fault and related interface energies in mechanical models (p. 129), quantum mechanical approaches to developing advanced

knowledge-based alloy design strategies and deriving mechanical property maps (p. 101, 133), and the connection of ground state energies and kinetic Monte Carlo simulations for predicting the early stages of precipitation phenomena in steels (p. 103).

Examples of our increasing interest in alloy design are the development of stainless quench-partitioning steels, age-hardenable Mn steels, Mg-Li and Mg-rare earth alloys, and complex FeAl-based engineering alloys (p. 105).

Scientific Groups

Introduction

The department has four regular scientific groups,

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

and four additional non-permanent scientific groups that are in part financed by third-party funds,

- Atom Probe Tomography (P. Choi)
- Computational Mechanics of Polycrystals (P. Eisenlohr)
- Theory and Simulation of Complex Fluids (F. Varnik)
- Intermetallic Materials (M. Palm, F. Stein)

Owing to their extramural funding the latter initiatives are temporary groups. The project of P. Eisenlohr on the Computational Mechanics of Polycrystals is 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 the Max-Planck-Institut and by 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 Intermetallic Materials originally was part of the department of Prof. Frommeyer and is currently closely cooperating

with us in the fields of high temperature materials, iron-aluminides, and Laves phases. In future it will be integrated into a new department.

Overview on permanent groups and their research focus in the past two years

Theory and Simulation (F. Roters)

Group Mission. The group mainly develops physics-based crystal plasticity constitutive models for the micromechanical behaviour of crystalline materials [1,7,9-13,41-48]. The models use coupled sets of lattice defect structure evolution equations that predict defect densities and the corresponding kinetic structure-property relations to translate the evolved structures into strength [1]. The constitutive laws assume a tensorial form both in their elastic and plastic formulations reflecting the underlying crystalline anisotropy of the material, i.e. they predict the defect evolutions on all crystallographic shear and twinning systems under external loads. This approach renders the constitutive models anisotropic. The formulations are built on mobile, sessile, and geometrically necessary dislocation populations, and can include mechanical twinning as additional deformation carrier (p. 129). 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) or a **Fast Fourier Method** (CPFFT) [1], Fig. 2.

Research Highlights 2009-2010. One important highlight in the past two years was the further development of the novel elasto-plastic 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 [1]. The main advantage of this approach is that FFTs can solve the underlying constitutive elasto-plastic equations under periodic boundary conditions about 2500 times faster than FEM solvers.
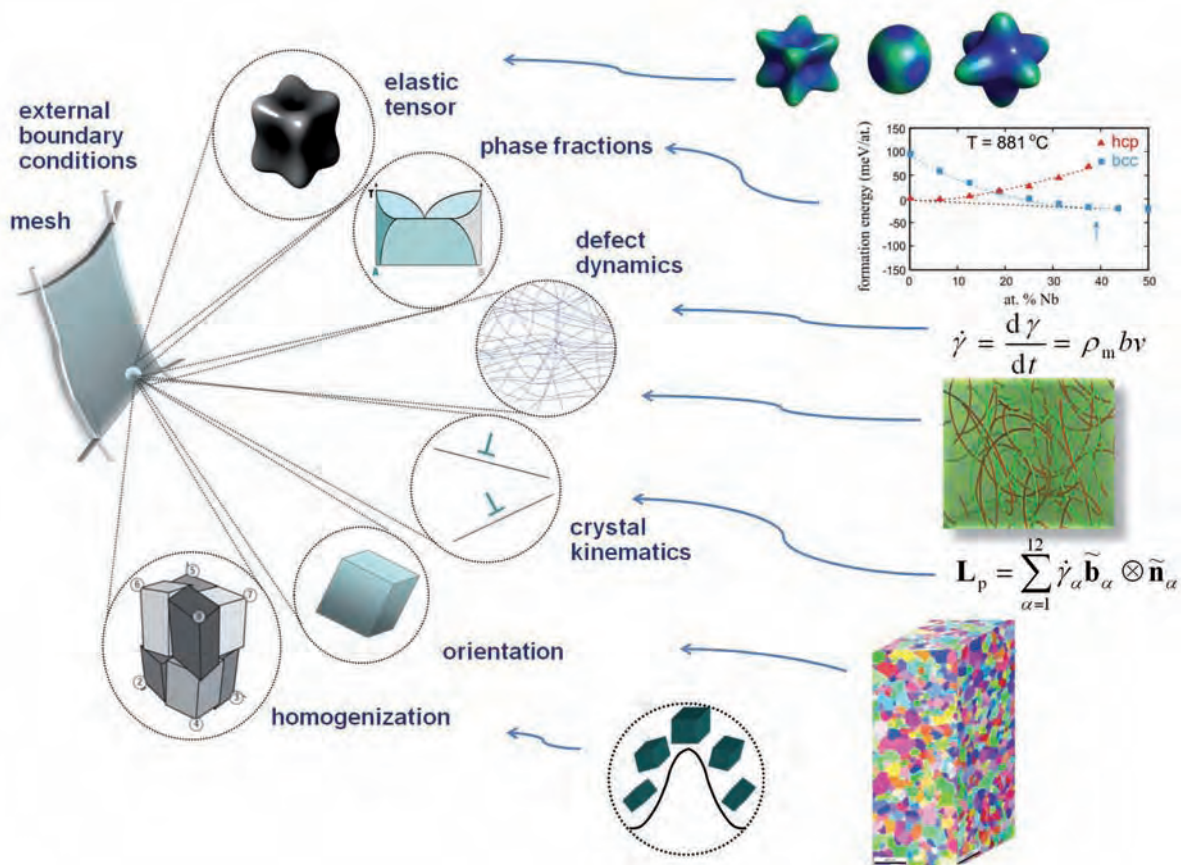
$$\dot{\gamma} = \frac{d\gamma}{dt} = \rho_m bv$$

$$\mathbf{L}_p = \sum_{\alpha=1}^{12} \dot{\gamma}_\alpha \tilde{\mathbf{b}}_\alpha \otimes \tilde{\mathbf{n}}_\alpha$$

Fig. 2: *Schematical diagram showing the most important constitutive input data and variables to internal-variable based crystal plasticity finite element solvers (the same applies to Fast Fourier solvers). γ: shear, b: Burgers vector, v: dislocation velocity, t: time, ρ_m: mobile dislocation density, n: slip system normal, L: velocity gradient. The dislocation populations are defined on each slip system (indices).*

Another field of activity was the application of advanced CPFEM simulations in conjunction with small scale mechanical experiments. A topic of high interest was the use of the CPFEM method to predict the orientation dependent pile-up and sink-in patterns obtained from spherical **indentation** testing (p. 109) [1,10,12,15,43]. Fitting of the simulations to the experiments can be used to extract slip system based constitutive strength and even strain hardening data from indents. This offers a large opportunity in using indentation testing beyond the determination of the reduced elastic modulus and the hardness.

A third field of interest are **discrete dislocation dynamics** (DDD) simulations. 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) [49] 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, Fig. 3 (next page).

The method is currently used in two directions. The first one is the discrete simulation of the early stages of strain hardening in bcc metals, specifically of the interaction between free lattice dislocations and low angle grain boundaries (dislocation walls). The second direction consists in systematic approaches to the coarse graining of these spatially discrete results and a corresponding knowledge transfer from discrete dislocation simulations to the statistical constitutive laws of strain-hardening that can be used in Crystal Plasticity FEM or FFT models. A coarse graining approach that is currently under development is based on dislocation density vector analysis.

Besides these simulations of the mechanical behaviour a **Cellular Automaton** (CA) program was developed that allows the simulation of industrial heat treatments of dual phase steels including recrystallisation as well as phase transformations.
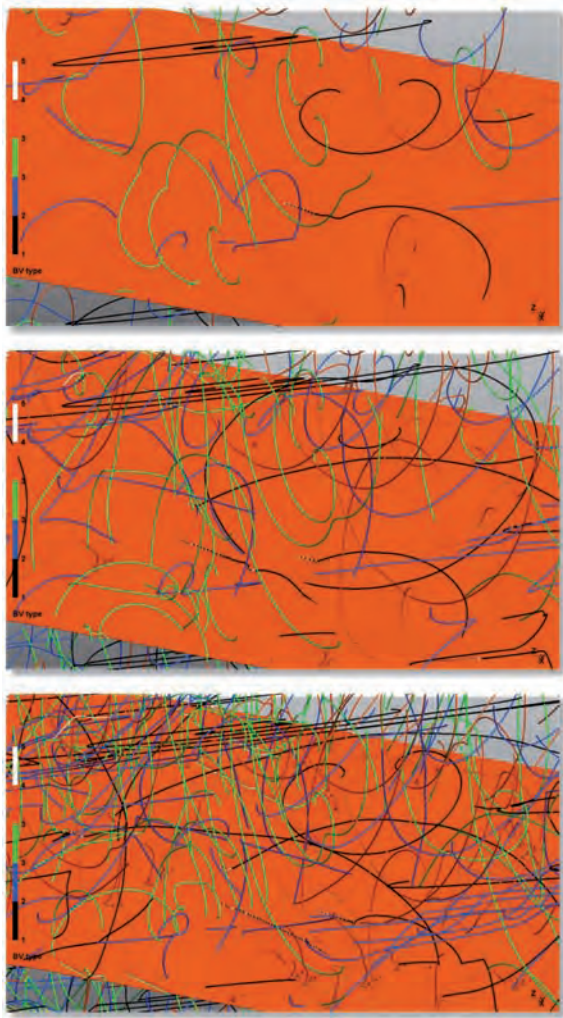
Fig. 3: *Discrete dislocation dynamics (DDD) simulations: Three subsequent snapshots of dislocation multiplication and structure evolution at a small angle grain boundary. The colour code indicates the Burgers vector of the dislocations.*

Microscopy and Diffraction (S. Zaefferer)

Group Mission. The group has two main missions. The first one is the development and optimization of new hardware techniques in conjunction with software tools for advanced microstructure characterization in TEM, SEM, and FIB-SEM instruments. Specific focus is placed on diffraction methods such as orientation microscopy in the SEM and TEM, **electron channelling contrast imaging** (ECCI), **internal stress** determination via SEM/EBSD, high resolution electron back scatter diffraction (HR EBSD), and 3D electron back scatter diffraction (**3D EBSD**, tomographic EBSD) [4-9,28,33,34].

The second main objective of the group lies in the application of these advanced methods with the aim to understand and quantify with high crystallographic precision microstructure evolution phenomena associated with a variety of thermal and athermal transformation mechanisms and the proper characterization of the interfaces involved. The phenomena pursued are mainly in the fields of crystal plasticity, recrystallization, grain growth, twinning, and TRIP (TRIP: transformation induced plasticity). Often the experiments are conducted on complex engineering multiphase materials [4,30].

The group operates several instruments. Among these is a Zeiss Crossbeam XB1560 FIB-SEM for 3D EBSD investigations, a JEOL JSM 6500 F SEM, and a JEOL JSM 840A SEM. These instruments are equipped with EBSD analysis hardware and allow mounting micro-deformation stages machines for in-situ deformation testing. A heating stage is also available for in situ transformation experiments. For TEM a Phillips CM 20 is used. This instrument is equipped with the software TOCA for on-line crystallographic analysis. Furthermore, several XRD goniometers are available.

Research Highlights 2009-2010. Highlight activities of the group during the past two years were the development of a quantitative approach to **electron channelling contrast imaging** (ECCI) [28,33]. This method improves the existing ECCI method in a way that it introduces the use of a preceding EBSD scan step and the subsequent calculation of the optimum sample tilting for obtaining good channelling contrast for the imaging of dislocation and interface substructures in the SEM (p. 107). This method offers huge opportunities for the fast quantification of substructure features at a large field of view that were not accessible so far to SEM characterization, Fig. 4. It can be combined with EBSD maps so that we are now capable of conducting detailed microstructure quantification mappings of orientation together with its inherent dislocation substructure in the same experiment [28,33]. 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 field of activity is the analysis of 3D EBSD data with respect to the characterisation of the interfaces via the crystallographic triangulation of corresponding grain boundary segments. The aim of this approach is to derive the five-parameter **grain boundary character distribution** (GBCD) function. This project is pursued in close cooperation with G. Rohrer and A.D. Rollett from Carnegie Mellon University, see Fig. 5 and p. 111.

Connected to this initiative is the focus that we place on software development in this field: The SEM and TEM based techniques mentioned above provide a high dimensional information vector of each probed crystalline point in a given microstructure including the local phase, crystallographic orientation, interfaces, curvature, internal stress state, dislocation substructure, and optionally also the chemical com-
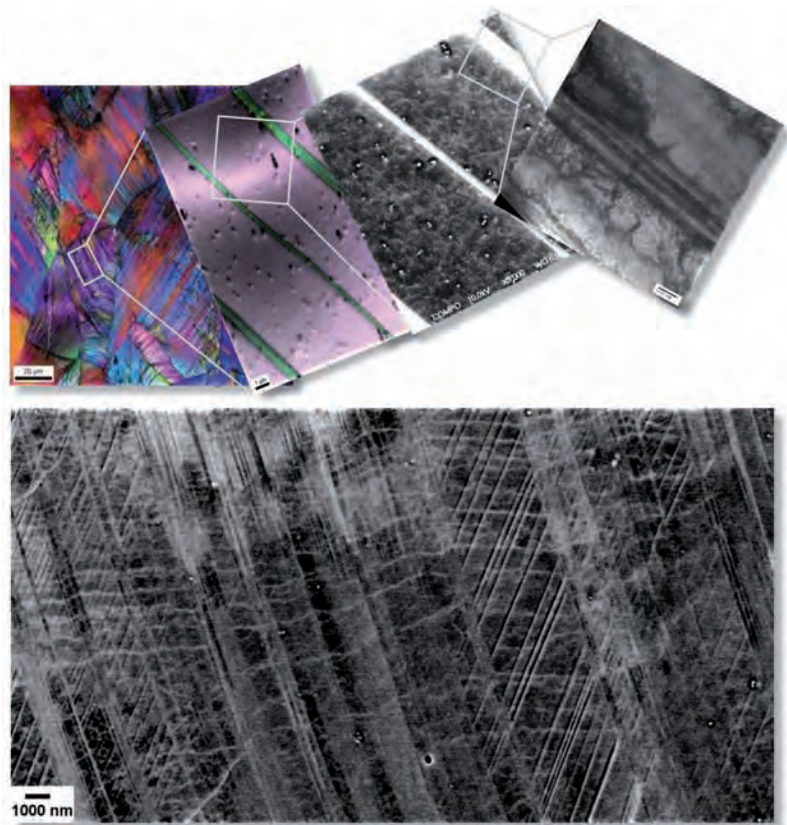
Fig. 4: *Upper row: Sequence of microstructure images of a deformed Fe-22 wt.% Mn TWIP steel obtained by EBSD (1st, 2nd), ECCI (Electron Channelling Contrast Imaging) in the SEM (3rd), and TEM (4th). Bottom row: Multiple twinning events in the same material observed at a large field of view in the SEM using ECCI [28,33].*

position via joint EDX maps. In order to extract meaningful information and particularly correlations (e.g. interface character distribution functions pertaining to a certain phase or texture component or the dislocation substructure of certain grains) it is required to develop corresponding software methods as particularly for tomographic EBSD methods commercial solutions do not exist.

A further recent focus of the group is placed on the development and use of SEM-based loading techniques for the in-situ observation of damage initiation mechanisms in crystalline materials. This is particularly used for the analysis of failure and strain localization effects in complex steels and titanium alloys. Another highlight during the past two years concerns the further improvement of the spatial resolution of the EBSD technique using low acceleration voltage.
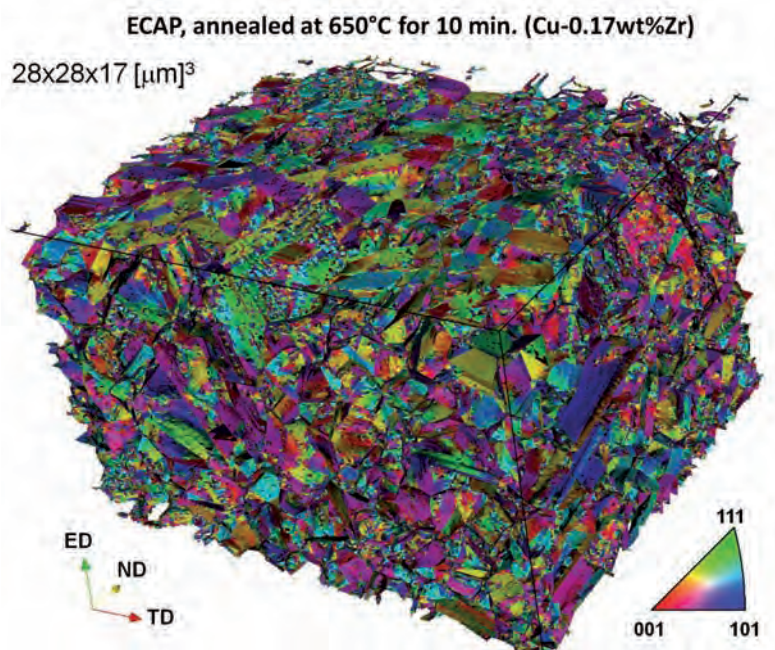
Fig. 5: *Example of the analysis of the grain boundary character distribution directly from 3D EBSD data taken on a highly deformed Cu alloy. The image shows from the 5 parameters that characterize the grain boundaries the normal vectors of the interface segments in terms of Miller indices using the standard triangle colour code.*
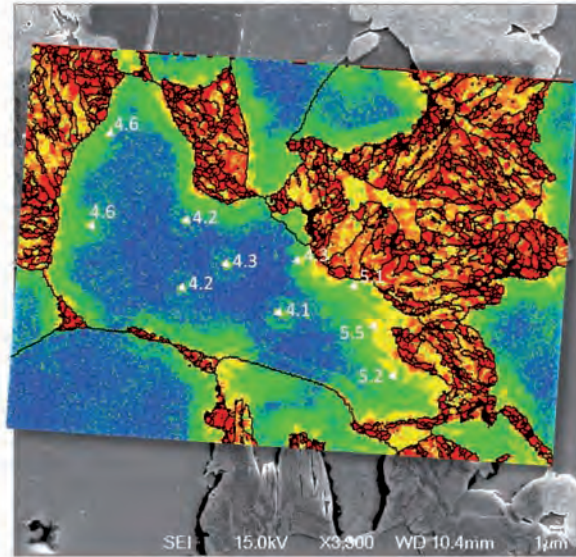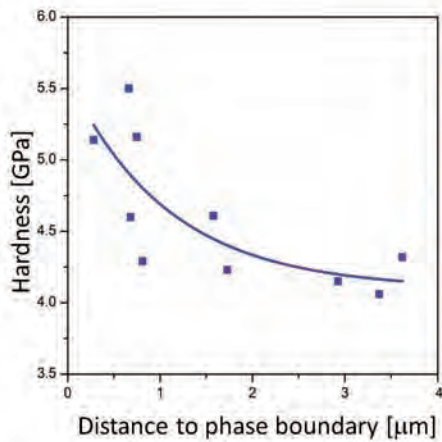
Fig. 6: *Hardness distribution in thermomechanically treated DP steel in front of the interfaces.*

Alloy Design and Thermomechanical Processing (D. Ponge)

Group Mission. The group's mission is the alloy design and subsequent microstructure-oriented optimization of properties of novel complex engineering steels via thermomechanical treatment [2,30-32]. This initiative requires a detailed understanding of the relations between processing and microstructure evolution on the one hand and the relations between microstructures and properties on the other. This two-fold strategy is essential in this field as no direct link exists between processing and properties. Hence, material optimization can only proceed through the careful characterization and interpretation of microstructures [30,42,50].

Fig. 7: *Atom probe tomography of nanoprecipitates in a Mn-based maraging-TRIP steel.*

The design of advanced thermomechanical processing pathways has up to now been the group's main objective in optimizing steel microstructures and hence their mechanical properties. Main examples from the past two years are the design of ultra fine grained steels placing attention particularly on plain C-Mn steels and dual phase (DP) steels for light-weight automotive applications [30,42,50], Fig. 6.

In addition to thermomechanical processing, projects increasingly include mechanism-based alloy design strategies [2]. The reason is that alloy development offers an ideal addition to thermo-mechanical 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 predictions tools and thermomechanical processing hence describes the current research strategy of the group (p. 103).

Research Highlights 2009-2010. Key projects in the past two years, related to thermomechanical process optimization, were mainly concerned with ultra fine grained **DP steels** [30,42,50] and DP **stainless steels** [41] where not only bulk micro-structures with a average phase size down to 1 µm were realized but also a detailed understanding of the interface-related strain hardening mechanisms was attained, Fig. 6.

A second direction was the development of a novel group of Mn-based lean **maraging-TRIP** steels [2]. Mn is an important alloying element in this context because it affects the stabilization of the austenite, the stacking fault energy, and the transformation kinetics [32]. While these effects are exploited particularly in designing steels with TRIP and TWIP effects (TRIP:
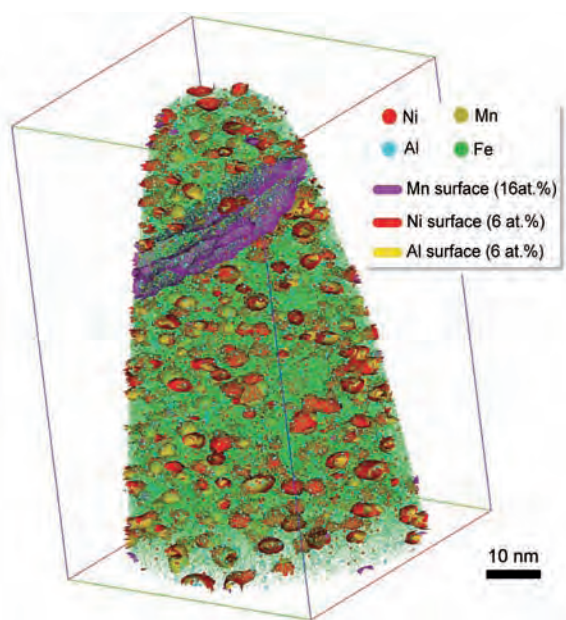
transformation-induced plasticity; TWIP: twinning-induced plasticity), the novel alloy concept introduced by the group combines the TRIP mechanism with the maraging effect (maraging: martensite aging) [2,32]. The TRIP effect exploits the deformation-stimulated transformation of metastable austenite into martensite, the resulting plasticity required to accommodate the transformation misfit, and the increase in the specific volume and the increase in strain hardening rate [38]. The maraging effect uses the hardening of the heavily strained martensite through the formation of nano-sized intermetallic precipitates during aging heat treatment, Fig. 7. The new maraging-TRIP steels reveal the surprising property that both strength and total elongation increase upon aging reaching an ultimate tensile strength of nearly 1.3 GPa at an elongation above 20% [2,38]. Due to the significantly reduced alloying costs in comparison to conventional maraging steels a wider range of applications can be addressed.

Biological Composites (H. Fabritius)

Biological materials are hierarchically structured nanocomposites optimized through evolution to perform vital functions within the specific eco-physiological strains of living organisms. Most biological materials with structural functions consist of an organic matrix of structural biopolymers like collagen, chitin or cellulose which is modified and reinforced with various other proteins and in many cases also with biominerals. The most prominent examples like the bones of vertebrates, the exo-skeletons of arthropods, and mollusk shells are known to possess excellent mechanical properties (e.g., in terms of stiffness-to-density ratio and fracture toughness) which are generated by structural and chemical alterations at different levels of their structural hierarchy. The origins of these properties, particularly the underlying structure-composition-property relations, are the research subject of this multi-disciplinary group.

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 [51-54]. Evidently, the overall properties depend on the specific microstructure at all levels of hierarchy. 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 our group in close cooperation with the department of J. Neugebauer to tackle the

structure/property relations of biological organic/inorganic nanocomposites. The method has in our group been applied to bone and lobster cuticle [23,51,53]. In addition to modeling fully differentiated structural composites, the approach has been successfully applied to model the mechanical properties of individual constituents and explain the structure/property relations on increasingly complex structural hierarchy levels [53-58]. A more detailed introduction to the new group and its current main fields of interest are given in a separate section (p. 18), see also p. 127.

Overview on non-permanent groups and their research focus in the past two years

Atom Probe Tomography (P. Choi)

Group Mission. The new group was opened in 2010. The opening ceremony was combined with an international workshop on the latest developments of atom probe microscopy. The research aims of the group and the laboratory equipment are introduced in more detail in separate sections (p. 16, 21). The main objectives of the group are in two fields. The first one is the near-atomic scale analysis of phenomena that mainly pertain to materials interfaces, such as segregation and partitioning effects and their consequences for the local thermodynamic and kinetic behavior [2]. The second one is the aim to compare atom probe tomography results 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 (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 since 2010. 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), Al- and Cr-Nitride multilayer hardcoatings, maraging steels, stainless steels, Ni-based superalloys, and metallic glasses.

The group is currently financed through the re-maining funds of Prof. Raabe's Leibniz Award (German Research Foundation, DFG). Owing to the excellent performance of the group during its first year of operation it is desirable that the shareholders provide additional funds to run the group in future on the basic budget.

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

Group Mission. The group was established in 2005 as the first ever joint research group between the Max-Planck-Society (Department of Micro-structure Physics and Metal Forming, MPI Düssel-dorf) and the Fraunhofer-Society (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg). Funding is 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 aerospace, automotive, and medical engineering (p. 33), Fig. 8.
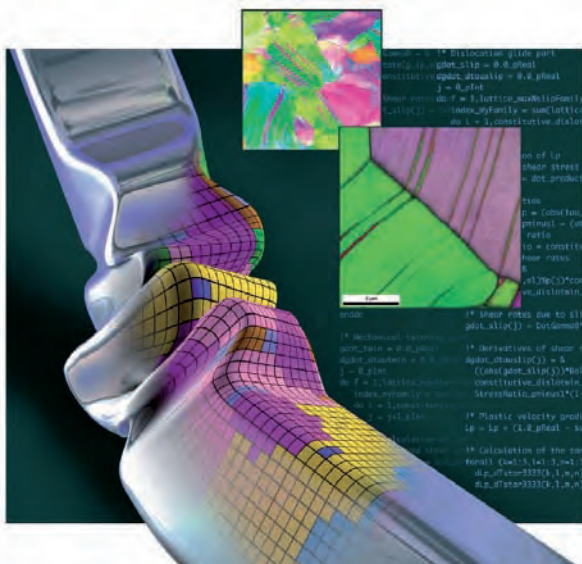
Fig. 8: *Schematical image showing to mission of the group, namely, the maturation of crystal plasticity finite element methods towards commercial applications.*

Research Highlights 2009-2010. In the past two years the group has pursued three main goals in close collaboration with the group for Theory and Simulation (F. Roters) [1].

The first aim was the development of an advanced grain or respectively phase cluster homogenization scheme [1,59]. 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. The current approach is referred to as Relaxed Grain Cluster model (RGC). 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.

The second aim of the group was the development of advanced constitutive models that describe the individual deformation behaviour inside the crystals [1]. Of particular interest was the development of constitutive models that include deformation twinning and its interaction with dislocation slip (p. 129).

The third area of interest was the role of hetero-geneous deformation on damage nucleation at grain boundaries in single phase metals [1,13,60]. 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, DFG, Materials World Network programme).

Theory and Simulation of Complex Fluids (F. Varnik)

Group Mission. The group, which is located both at ICAMS and at the Max Planck Institute, studies the mechanical properties of complex multiphase and colloidal fluids. In many cases, such fluids are easily deformed under the action of rather weak forces such as in the case of shear melting. This effect is often accompanied by a drop in shear viscosity upon increasing shear rate (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 the soft matter processing industry, in biology, and in metallurgical casting and solidification processes [61,62]. As a modeling tool, the group uses the lattice Boltzmann method (LBM) and multiphase variants thereof [63-69]. LBM is a powerful tool 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 because it has high computational efficiency, good versatility in the constitutive description of its pseudo-particles, and simplicity in coding. 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 [61,62].

Research Highlights 2009-2010. Using the LBM, the group investigates problems in micro-fluidics such as inhomogeneous diffusive broadening [66], droplet and contact dynamics on chemically [64] and topographically [67,68] patterned substrates as well as flow between topographically rough walls [63,64]. 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 multiphase LBM variants that are recently particularly used for the study of blood flow mechanics [65,69]. 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 prediction of genuinely new wetting states in the case of small droplets with a size comparable to the roughness scale [67,68].

Intermetallic Materials (M. Palm, F. Stein)

Group Mission. Fundamental research on phase stability and phase transformations of intermetallic phases and establishing properties to elucidate the possibilities of their industrial application are the two aims of the Intermetallic Materials group.

A sound knowledge of the phase equilibria in dependence of composition and temperature is the basis for any kind of materials development. For intermetallic materials this information is often lacking, which is partly due to considerable experimental difficulties in investigating these high-melting materials. Therefore, besides metallography, XRD, EPMA and DTA, additional methods such as *in-situ* neutron diffraction [70,71] and advanced TEM techniques are employed [72,73]. In addition, the diffusion couple technique is widely used for a rapid study of phase equilibria [74,75]. In order to evaluate the potential for industrial application, fundamental mechanical properties such as hardness, yield strength and creep resistance and the basics of the oxidation behaviour in air are studied [76].

The group has tight connections with the neighbour departments, especially on the topics of *ab-initio* thermodynamics [77,78] and corrosion [79], and multiple international collaborations [70,71,73,74,80,81]. The development of intermetallic materials for structural applications is performed in close cooperation with industry [82].

Research Highlights 2009-2010. Currently, Laves phases and Fe and Ti aluminides are the main topics of research. The stability of the different crystallographic structures of the Laves phases in dependence on temperature and composition and their effect on mechanical behaviour are studied in detail (p. 93). For Fe-Al-based materials a long lasting problem has been solved with the determination of the crystallographic structure of the high-temperature phase ε (Fe_5Al_8, cubic, space group I-43m) [83]. In view of the practical application of Fe-Al, considerable progress was obtained by the development of a forging route [82] and the characterisation of the microstructure and mechanical properties in different parts of a forged steam turbine blade [84]. Within the framework of a larger programme, the complex phase transformations and resulting mechanical properties of Al-rich Ti-Al alloys have been investigated [72,85]. These TiAl + Al_2Ti alloys offer a reasonable creep resistance, especially in view of their low density (3.8 g/cm^3) and in that they show an improved oxidation resistance compared to established TiAl alloys. However, even generating lamellar TiAl + Al_2Ti microstructures only results in a minor increase in ductility of these rather brittle materials.

Main Laboratories of the Department

The main laboratory facilities of the department are

- Atom probe tomography (LEAP)

- TEM and Atom probe sample preparation laboratory via SEM-FIB dual beam (FEI Helios)

- Micro- and macro-mechanical testing laboratory from micro- to centimeter length scales

- High resolution scanning orientation electron microscopy (Jeol, Zeiss)

- 3D electron microscopy: Joint SEM-FIB microscopy and 3D nanotexture laboratory (Zeiss)

- Transmission electron microscopy laboratory (Jeol, Philips)

- X-ray diffraction laboratory (Bruker, Philips)

- Strain mapping digital image correlation (photo-grammetry) laboratory

- Surface confocal topography laboratory

- Nanomechanical testing and atomic force microscopy laboratory (Hysitron)

- Laboratory for deformation dilatometry

- Computational materials science laboratory

- Large scale thermomechanical treatment laboratory, hot and cold rolling, heat treatment

- Optical metallography laboratory

- Liquid metallurgy and casting laboratory

Main Interdisciplinary Research Fields

The objectives of the research groups and their core competences were described above. A number of further key projects in the department are jointly pursued by members of different groups including also other departments. More specific scientific details about some of these inter-departmental and inter-disciplinary projects are given in the research highlight section. The following paragraphs introduce some main current inter-disciplinary research topics in the department.

Mechanism-oriented and knowledge-based alloy design

The design of **novel alloys**, mainly structural alloys in our case, is a key challenge in the field of materials science for four main reasons.

First, thermomechanical processing for the de-sign of beneficial microstructures is an efficient but limited approach. Including a higher variety of possible solid solution and phase transformation phenomena by chemical alloy modifications opens the field of materials design far beyond the scope offered by processing alone. On the other hand, introducing new compositions without systematic thermomechanical treatment studies does also not provide sufficient depth in structural alloy design. Hence, the two disciplines are increasingly merged in our department.

Second, alloy development is nowadays conducted not only for the mass market but increasingly for very specific applications. This means that new materials are not necessarily designed for a wide spectrum of possible applications but rather for an application niche with high profits.
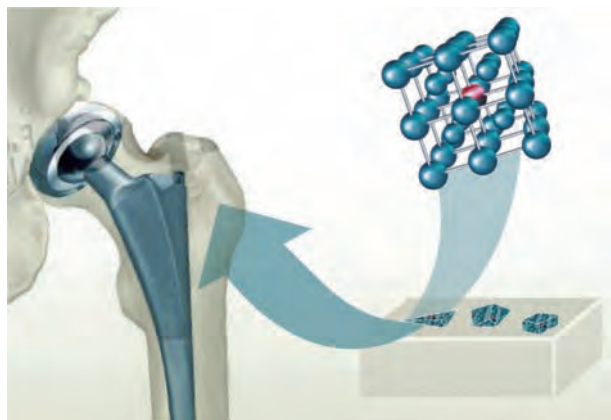
Fig. 9: *Schematical sketch of an ab initio strategy for designing elastically soft bcc Ti-Nb alloys. First the elastic constants are calculated for different compositions and lattice structures (bcc, hcp) by DFT (Density Functional Theory). Second, the elastic constants are used for polycrystal homogenization via FEM or FFT methods [18,20,21,25].*

Third, the use of novel theoretical tools such as *ab initio* simulations (department of J. Neugebauer) and kinetic Monte Carlo methods in conjunction with established thermodynamic and kinetic simulation tools such as **ThermoCalc** and **Dictra**, render the field of alloy design increasingly accessible to quantitative predictions [2].

Fourth, high throughput alloy design methods have provided considerable success in the fields of functional alloys. Corresponding methods are not yet readily transferable to structural alloys which require at least a critical probed volume fraction above a multiple integer of the grain size and an intermediate forming and heat treatment step.

For these reasons we have in the past two years increasingly shifted our activities in **thermo-mechanical processing** towards including **alloy design** (mainly in the group of D. Ponge, in col-laboration with the department of J. Neugebauer). Examples of joint alloy design and thermomechanical treatment studies are the development of a new class of Mn-based maraging-TRIP steels (p. 105) with more than 20 chemical variants and hundreds of different heat treatment variations, high C (>0.3 wt.% C) quench-partitioning stainless steels with 13 wt.%Cr; Fe-3wt.%Si-Cu steels for applications in electrical engines (p. 103); Mg-Li alloys; Mg-rare-earth alloys; Cr-Mo-Fe-Co dental alloys; bcc Ti-Nb materials, Fig. 9; and Ti-alloys with different sets of solid solution ingredients including Mo, Nb, V, and Al. Exiting and unexpected results were particularly obtained on the new Mn-based maraging TRIP steels, where we observed - unlike for conventional maraging steels - the increase of both, strength and toughness upon aging heat treatment (p. 105). In all cases ThermoCalc simulations have been used. For specific systems such as Fe-Mn, Ti-Nb, Ti-Mo, Mg-Li, Mg-rare earth, Fe-Si-Cu, and Fe-Cr-C *ab initio* simulations are conducted by the department of J. Neugebauer.

The Crystal Plasticity Fast Fourier Transform (CPFFT) Simulation method

Full-field direct Fast Fourier Crystal Plasticity methods solve the equilibrium and compatibility constraints for anisotropic elastic or elastic–plastic polycrystal and polyphase problems using the Fast Fourier Transformation approach [1]. The discrete Fourier approach renders the governing set of crystal elasticity and plasticity differential equations into a discrete algebraic problem which can be solved much faster than the conventional weak-form variational approach used by the Finite Element method. In order to use discrete series expansions, spectral methods have to use a fixed grid and a representative cell arrangement of the microstructure considered. Discrete Fourier formulations imply periodicity of the
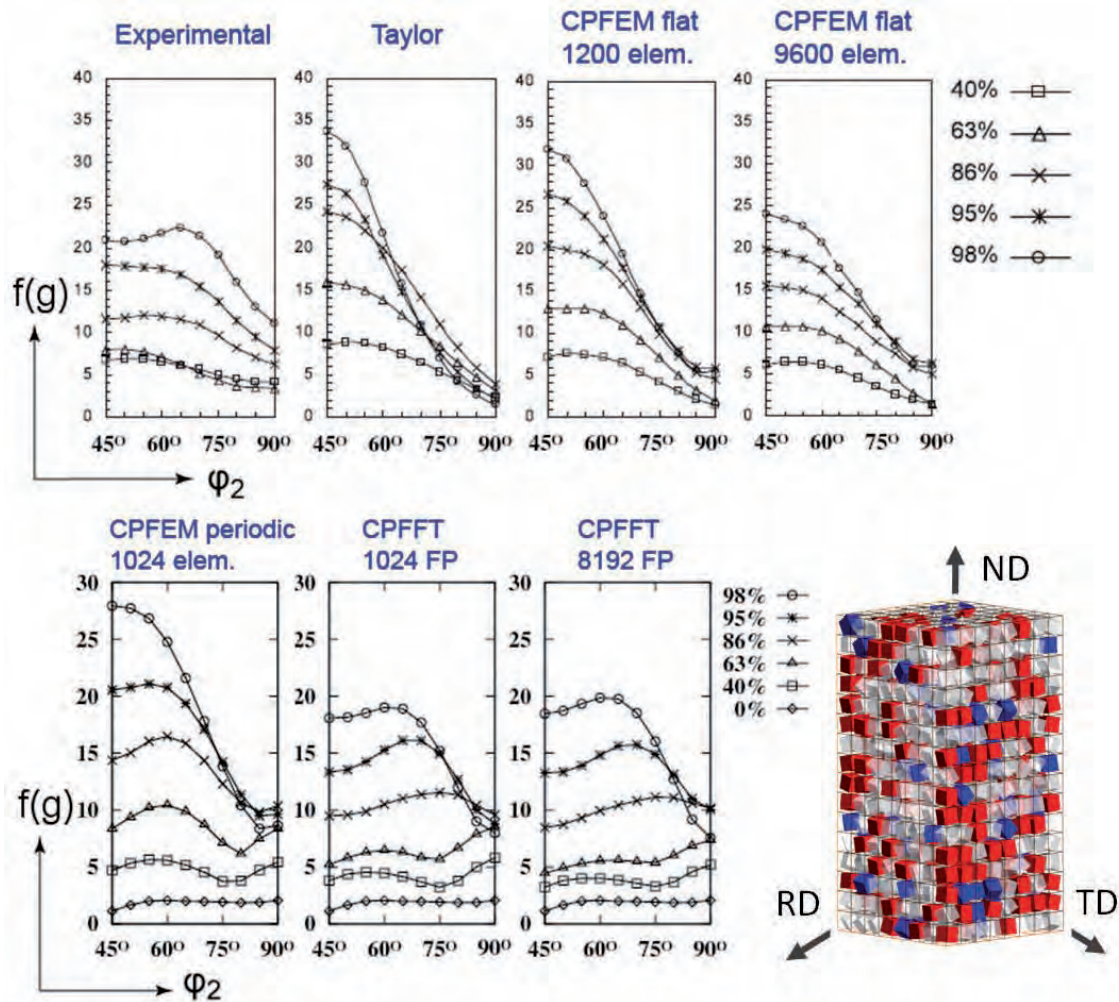
Fig. 10: *Rolling texture evolution. The upper row shows results from the literature of Li et al. [86] for the fcc lattice structure: Experimental results of an aluminium alloy AA1200; Taylor model; CPFEM model with flat surface conditions (1200 elements, 1200 grains); CPFEM with flat surface boundary conditions (9600 elements, 1200 grains). The bottom row shows rolling texture predictions obtained in our group: CPFEM with periodic boundary conditions (1024 elements, 1024 grains); CPFFT (1024 Fourier points, 1024 grains); CPFFT (8192 Fourier points, 1024 grains). The crystal distribution on the right hand side indicates the starting texture (weak cube texture). The FFT solution yields excellent texture predictions and is about 2500 times faster than the FEM solver.*

modeled aggregate. Since the displacements lead to state values between the fixed coordinates of the discrete Fourier set-up, interpolation functions must be used.

During the past two years it has been a core project of the department to combine advanced **internal variable** based constitutive strain hardening laws with a novel anisotropic Fast Fourier Solver with the aim to introduce a **Crystal Plasticity Fast Fourier Transform (CPFFT)** method as a new simulation method into the field of crystal mechanical research. The work was conducted as a collaboration of the groups of F. Roters and P. Eisenlohr with R. Lebensohn from Los Alamos National Laboratory, USA, who spent a year in the group as an Alexander von Humboldt Awardee. A versatile CPFFT software package was developed during this cooperation which is now capable of using the same variety of constitutive strain

hardening formulations (viscoplastic, dislocation-based, strain-gradients, interfaces, deformation twinning) as the well established Crystal Plasticity Finite Element (CPFEM) solvers that are used as a main mechanical simulation method so far in the department. The main advantage of the new CPFFT approach is that it can solve the underlying constitutive elasto-plastic equations - under periodic boundary conditions - about 2500 times faster than CPFEM solvers. Also CPFFT has the advantage that it can directly be applied to EBSD or other fixed-grid microstructure data sets without the necessity to reconstruct complicated mesh geometries as it is required for CPFEM simulations. As one classical benchmark test we compared the two full-field crystal mechanical formulations (CPFFT, CPFEM) in terms of the plane-strain deformation textures predicted by both approaches. The predictions showed excellent agreement with each other and with experimental results, Fig. 10.

Multiscale modeling based on *ab initio* predictions: From descriptive to predictive simulations

In a number of projects we develop multiscale materials simulation approaches that are based on *ab initio* models. The electronic and atomistic predictions are conducted in the department of J. Neugebauer and the continuum theoretical and homogenization aspects are pursued in our department [1]. Besides the different theory groups a number of experimentalists (electron microscopy: S. Sandlöbes, S. Zaefferer, H. Fabritius, A. Kostka; atom probe tomography: P. Choi, O. Dmitrieva) and alloy design experts (D. Ponge) are involved as in all projects we aim at a detailed comparison between predictions, experiments, and alloy synthesis.

Currently we pursue joint multiscale modeling project in four main fields. These are theory-guided and mechanism-oriented **alloy design**; coarse graining and **homogenization** methods; design and experimental analysis of Ashby-type mechanical **property maps** based on *ab initio* predictions; and the analysis of **interfaces** and **twinning** phenomena such as occurring in Fe-Mn steels, Al, and Mg alloys.

In the field of alloy design we predict basic thermodynamic and kinetics quantities on the one hand and microstructurally relevant parameters such as the alloy-dependence of stacking fault and related interface energies on the other hand. The former approach (thermodynamics, kinetics) is applied to the early precipitation stages of Cu–nanoparticles in Fe-3wt.% Si as soft magnetic alloys for electrical engine applications; to the energy landscape of $(Fe,Cr)_{23}C_6$ carbides with different Fe-Cr compositions in stainless steels; and to Ti-Nb and Ti-Mo low-stiffness alloys with bcc lattice structure for biomedical implants. The latter approach (compositional changes in the deformation mechanisms) is applied to the Fe-Mn, Mg-Li, and Mg-rare-earth systems, placing attention particularly to the prediction to the variation in the stacking fault and related interface energies as a function of the chemical composition and their promoting or inhibiting effects on deformation twinning and dislocation cross slip phenomena relative to other plastic degrees of freedom.

Another field of interest in multiscale modeling is the homogenization of elastic (and other tensorial) properties that are calculated for the single crystal state by *ab initio* methods. As polycrystalline and polyphase materials constitute crystalline aggregates of arbitrary crystallographic orientation distribution the calculation of the macroscopic properties of the entire specimen requires an averaging or even a full-field homogenization scheme. For instance, for the case of non-random crystal orientation distributions and linear elastic problems classical upper or lower bounds can be estimated by Voigt (iso-strain) or Reuss (iso-stress) estimates. More complex and realistic internal loading cases can be captured by the self-consistent Eshelby scheme or by full-field Crystal Elasticity Finite Element or Fast Fourier integration methods [1], Fig. 2. Areas where we use such schemes are the repeated hierarchical homogenization of the elastic stiffness of biological materials, more specific, of the stiffness of the exoskeleton of arthropods [51]. Another application is the calculation of the polycrystal Young's modulus of bcc Ti-alloys and Mg-Li alloys.

The third branch of *ab initio* based multiscale models pursues the design of engineering Ashby-type property maps for Al-, Ti-, and Mg alloys [16,18-21,25]. The aim is to derive measures that describe the macroscopic mechanical response of alloys as a function of chemical composition and electronic trends directly – i.e. without complex intermediate simulation steps – from **ab initio** simulations. An example is the calculation of the specific elastic stiffness of the material (Young's modulus divided by mass density) as a function of the ratio between the hydrostatic bulk and the shear modulus. The latter quantity describes the resistance of the material against rupture normal to a lattice plane (hydrostatic bulk modulus) normalized by its resistance lateral to a lattice plane (shear modulus). Materials that can be easily sheared but have high bulk stiffness are less brittle and more ductile as opposed to those that have a low bulk modulus and a high shear modulus.

The fourth field aims at using *ab initio* derived interface energies directly as constants in constitutive plasticity laws. An example is the use of composition-dependent stacking fault energies in strain hardening formulations of TWIP steels.

Understanding the strengthening mechanisms in ultra high strength steels

The design of materials towards their respective limits of strength is one the grand basic aims in mechanical materials science. While the theoretical strength limit is determined (for Whiskers) by the rigid shear of two parallel lattice planes (can be estimated by G/50, where G is shear modulus), real materials contain lattice defects that lead to much lower stress values of the critical shear, strain hardening, and failure. The design of real engineering materials towards ultra high strength levels thus requires a detailed understanding of the strain hardening mechanisms that impede dislocation motion.

Metallic materials, when exposed to external mechanical loads, go through a sequence of complex microstructure refinement phenomena that can be exploited to increase their strength by several orders of magnitude. These are at intermediate stress levels the Hall-Petch-type interface hardening which limits the mean free dislocation path. At high defect densities (dislocations or interfaces), conventional bulk plasticity becomes less relevant for the further increase in strength. This means that dislocation–dislocation interactions within the constituent phases and the Hall-Petch effect are gradually replaced by limitations in activating dislocation sources, by dislocation reactions at the hetero-interfaces, and by Orowan expansion of dislocations within confined volumes.

Upon further microstructure refinement, dislocation (hetero- or homophase) interface penetration effects start to occur. Such heterophase slip transfer effects do most likely not only occur in the form of single slip transition effects but also in the form of localization effects across interfaces by micro- or shear bands. When the microstructure refinement reaches a level where intraphase dislocation multiplication and motion becomes geometrically impeded, slip transmission across the hetero-interfaces starts to gain momentum.

One essential observation that is common to all heavily deformed metallic multiphase alloys is the phenomenon of mechanical alloying. This means that multiphase materials with limited mutual solid-state solubility undergo plasticity-stimulated chemical mixing to levels far beyond equilibrium solubility. In many cases this phenomenon even leads to the complete dissolution of the minority phase into the matrix phase. Another mechanism that occurs at high strains is that some systems undergo deformation-driven solid-state amorphization.

In our current projects on ultra high-strength steels we particularly pursue two strategies, namely, the increase in the interface homophase and heterophase density through thermomechanical processing and alloying effects (nano-precipitates) and the design of materials with increased forced solid solution content through quench-partitioning treatments and deformation-stimulated mechanical alloying.

The former method is realized in ultrafine grained DP steels with well tailed grain sizes down to 1 µm, Fe-Mn based maraging-TRIP steels which contain complex nanoparticles through martensite aging, and TWIP steels with a high density of deformation twins. The latter approach is realized in pearlitic steel wires where we reached an ultimate tensile strength of 6.5 GPa and Fe-Cr quench-partitioning steels with a carbon content above 0.3 wt.%.

Multiphase tomographic 3D EBSD and 5D GBCD analysis

In the past two years we have further refined the tomographic microstructure and texture analysis method via the 3D EBSD approach [4-8]. This method is realized by fully automated serial sectioning as a combination of a focused ion beam (FIB) system and EBSD in a high resolution field emission SEM. The sectioning by FIB provides an accurate depth definition, yields flat and parallel sections (< 1° deviation), and high resolution (< 50 nm). The subsequent EBSD mapping of each slice provides a well-defined contrast on crystalline material including a variety of different phases, a fully quantitative description of the microstructure at high resolution (~ 50 nm), and a high measurement speed. The system runs fully automatic. Further details of the 3D method were discussed in more detail in the last scientific report.

We currently shift our activities in this field from the mere 3D texture analysis to the additional mapping of the full crystallography of the interface segments between the grains (3 misorientation parameters and 2 interface plane parameters). This field is referred to as the analysis of the **grain boundary character distribution** (GDCD) function, Fig. 5. Grain boundaries play an essential role in many transformation, segregation, corrosion, deformation, and damage processes. As the structure and properties of the grain boundaries vary in a 5-dimensional parameter space it is important to systematically characterize and investigate the GBCD in crystalline materials exposed to different thermomechanical pathes (p. 111).

Mechanical properties at micrometer-scales

As current trends towards device miniaturization accelerate, the micro-mechanical characterization of materials becomes increasingly important. Mechanical properties and the underlying plasticity mechanisms at dimensions below 20 µm differ from those at the macroscopic scale (smaller-is-stronger). Often, an inverse relationship is observed between the sample size and the flow stress. This applies even for compression tests under gradient-free loading conditions [7,8,11,12]. Mechanical tests at such small scales are not only characterized by their sensitivity with respect to the initial microstructure and specific size dependent deformation mechanisms (intrinsic size effects) but also by an increasing relative influence of the experimental initial and boundary conditions on the results (extrinsic size effects). The latter point has been studied by the group in terms of sample shape variations, contact,
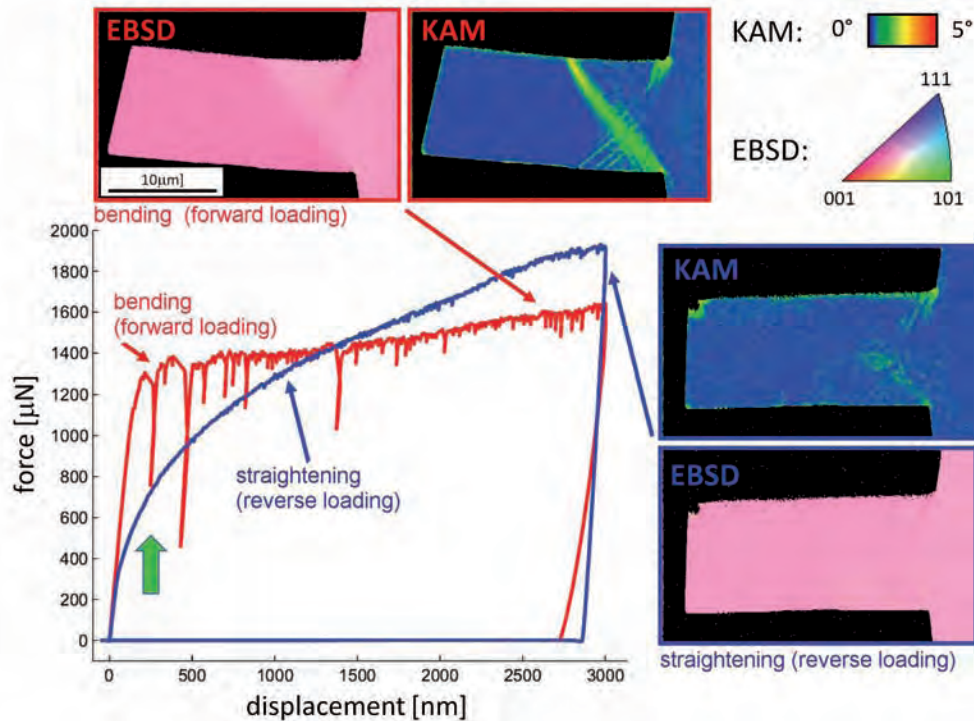
Fig. 11: *Force-displacement curves of the first bending (red) and straightening cycle (blue) together with the complete microstructure maps (EBSD: Electron back scatter diffraction; KAM: Kernel average misorientation). The green arrow indicates a load drop where a strain burst occurs [87].*

loading procedures, appropriate criteria to define the onset of plastic flow, and Bauschinger effects (path dependence of flow stress), Fig. 11.

Intrinsic (microstructural) effects that are typically held responsible for the smaller-is-stronger phenomenon are geometrically necessary dislocations (GNDs) and pile-up effects [11,12]; dislocation starvation [12]; and dislocation source truncation [12]. The scaling of the yield stress with probe size is different for these mechanisms. While GND-related strengthening leads to power-law exponents close to -0.5, source limitation effects would show an exponent close to -1. All these models assume a mean-field behaviour of the dislocations. Plastic deformation below the statistical regime (mean-field break-down), however, is characterized by substantial deviations from the average dislocation behaviour and hence, by large scatter in the observed flow stress. This makes it difficult to assign one single mechanism to the observed size effect. The same argumentation applies when in a sequence of smaller-is-stronger experiments transitions between different deformation mechanisms take place. This can be particularly expected when probe sizes below and above characteristic microstructural length scales are used.

In order to elucidate these points we conducted several types of microscale bending tests of single slip oriented copper single crystal beams and conducted subsequent EBSD characterization. The measured flow strength values were size dependent. The yield strengths depended not only on the beam thickness but also strongly on the yield criteria selected. Changing the critical threshold strains for flow begin could alter the flow stress values by several 100% for the smallest beams. As reason for this effect we identified the size dependence of strain hardening. The analysis, hence, revealed, that the contribution of strain hardening to the smaller-is-stronger phenomenon is more important than the incipient size dependence of the flow strength observed at the onset of plastic straining. Geometrical inaccuracies may significantly influence the resulting microstructure by causing stress concentrations. The effect of these inaccuracies on the microstructure was mapped using EBSD, Fig. 11.

Also we observed that the yield strength size effects estimated from the GND densities that were obtained from misorientation maps alone did as a rule not explain the observed phenomena. For fully explaining the observed smaller-is-stronger effects we hence introduced a microstructural mean-field break-down theory and generalized the idea to small scale mechanical tests. According to this approach the mean-field break-down limit is defined by a microstructural correlation measure (characteristic bow-out length) below which the local availability of dislocation sources and not the density of GNDs alone determines the mechanical size effect. According to our estimates most small-scale bending experiments can be interpreted in terms of this theory [11].

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 physics, materials science, metallurgy, biology, informatics, chemistry, and mechanics, Fig. 12. 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.

The working atmosphere was during the past 2 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, Nigeria, Romania, Russia, Sweden, Spain, Poland, The Netherlands, Turkey, UK, Ukraine, USA, and Venezuela. Our international orientation is also reflected by our extramural cooperation partners, namely, Prof. Bleck, Prof. Schneider, Prof. Dronskowski, and Prof. Gottstein (RWTH Aachen, Germany), Prof. Rollett and Prof. Rohrer (Carnegie Mellon University, USA), Prof. Lebensohn (Los Alamos National Laboratory, 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).

Fig. 12: *The team.*

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Research Projects in Progress

Choi: Thermal stability of metal nitride superlattices studied by means of atom probe tomography

Davut, Elhami, Zaefferer: Relationship between microstructure and damage mechanisms in multi-phase steels

Dmitrieva, Choi, Raabe, Hickel, Neugebauer: Analysis of the kinetics of precipitation in Fe-Si-Cu at the atomic level using atom probe tomography

Dmitrieva, Raabe: Deformation-induced orientation laminates and orientation patterning in single crystals

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

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

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

Jäppel, Zaefferer: Local strain determination in Mn-based steels

Khorashadizadeh, Raabe, Winning: Mechanical properties of ultra-fine grained materials

Krüger, Varnik, Raabe: Blood flow mechanics

Ponge, Raabe, Herrera: Ductile high nitrogen duplex stainless steels

Prymak, Dmitrieva, Raabe: Limits and influences of impurities in Titan-recycling alloys

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

Raabe, Neugebauer: Multiscale materials modeling of condensed matter

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

Raabe, Winning: Fast agorithms for materials-oriented process simulation in metal forming

Raabe, Zaefferer: Fundamentals of soft magnetic FeSi transformer steels

Raabe: Mechanics of phase boundaries in multi-phase steels

Roters, Eisenlohr, Raabe, Lebensohn: Computational mechanics of polycrystals

Sandlöbes, Zaefferer: 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

Stein, Palm, He (Guangxi University, China): Liquidus surfaces of the ternary systems TM-Al-Nb (TM = Cr, Fe, Co)

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

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

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

Varnik, Raabe: Non-equilibrium flow at gradient surfaces: multi-component fluids

Voss, Stein, Palm, Raabe: Mechanical properties of Laves phases

Yuan, Ponge, Raabe: Forming properties of ferritic Cr steels

Zaefferer, Elhami: Characterization of the microstructure and deformation mechanisms in TWIP-(X-IP u. L-IP) steels

Zaefferer: In-situ SEM-analysis of three-point bending tests

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Max Planck Fellow Research Group on High Temperature Materials

A. Kostka, G. Eggeler

Background

There is a continual drive for increased thermal efficiency in energy conversion and aircraft propulsion systems. Therefore operating temperatures have been progressively increasing during the last decades. Critical high temperature components like steam headers in coal fired power plants or first stage blades in advanced gas turbines are manufactured from high temperature materials which possess a high inherent creep strength in combination with a good high temperature corrosion resistance. Tempered martensite ferritic steels (600°C range), high temperature austenitic steels (700°C range) and single crystal super alloys (1000°C range) represent examples for high temperature engineering materials which receive considerable attention. High temperature materials researchers also take interests in intermetallic materials like TiAl or FeAl and other metallic systems like Mo-Si-B, Co-Re or Co-Al-W-Ta.

High temperature materials are not only technologically interesting. They represent a fascinating subject area for research in different fields of materials science and engineering. They are usually difficult to process and manufacture. Therefore basic research on processing technologies like ingot metallurgy or welding is important. High temperature materials generally have complex microstructures and therefore a good understanding of thermodynamic stability and of microstructural evolution during high temperature service is required. There is a need to use optical microscopy, scanning electron microscopy and transmission electron microscopy (with the advanced extensions available today like orientation imaging in the SEM or electron loss spectroscopy in the TEM) in combination with quantitative image analysis to investigate microstructures. And today the 3D atom probe method allows to chemically analyse volumes of 1 μm^3 which are large enough to study elementary diffusion reactions in high temperature materials. In mechanical high temperature testing there is an interest in new test procedures for a better characterization of creep and high temperature fatigue. It is important to be able to address creep under multiaxial stress states, to characterize creep and high temperature fatigue crack growth, thermal fatigue and miniaturized specimen geometries are in the focus of interest. It is important to have good mechanical and microstructural data for input and validation purposes in order to understand and model the interaction of elementary deformation and damage processes which govern the behaviour of critical high temperature components. Moreover, research on high temperature materials strongly benefits from progress in advanced materials modelling on all length scales.
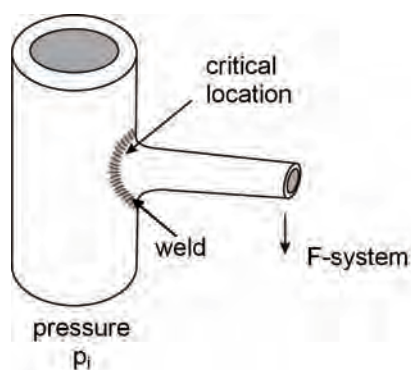
Fig. 1: *Schematic illustration of a creeping T-piece (a critical high temperature component in a steam boiler).*
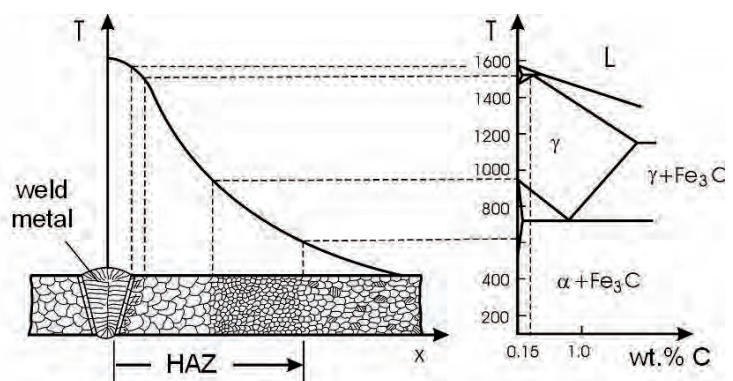
Fig. 2: *Schematic illustration of how welding affects the local microstructure of a hypoeutectoid steel.*

Fig. 3: *Miniature tensile creep specimens taken from a tempered martensite ferritic steel tube.*

Scientific Objectives

We take a broad view on materials science and engineering of high temperature materials focussing on interesting mechanical, chemical, microstructural and theoretical topics. We take interest in all aspects of processing, manufacturing, microstructure evolution, high temperature properties and applications of traditional and new high temperature materials. The group explores strategies for the development of new high temperature alloys, for the improvement of existing materials and for the improvement of high temperature joining procedures. The effect of joining on local microstructure and strength is in the focus of interest. The High Temperature Materials (HTM) group investigates elementary mechanisms which govern high temperature strength of complex engineering materials. The group has expertise in creep testing, high temperature fatigue testing and combines high resolution mechanical experiments with analytical scanning and transmission electron microscopy and with quantitative analysis of micro-structures. The group performs research on (i) the influence of grain boundary crystallography and chemistry on creep cavitation, on (ii) elementary deformation and damage process during creep of short fibre reinforced Al-alloys, on (iii) dislocation reactions in single crystal Ni-based superalloys and on (iv) interdiffusion processes associated with joining of dissimilar materials (like e.g. Al and Fe) and their effect on microstructure and mechanical properties. The group closely interacts with all departments of MPIE and acts as an operational link between the high temperature activities of G. Eggeler's Chair for Materials Science and Engineering (Lehrstuhl Werk-stoffwissenschaft at the Ruhr-Universität Bochum) and the MPIE. Within the group, A. Kostka (group leader of the HTM group) and G. Eggeler (Max Planck Fellow) continue their successful collaboration which started with a two-years postdoc period which A. Kostka spent at the Ruhr-Universität Bochum prior to joining MPIE in 2007.
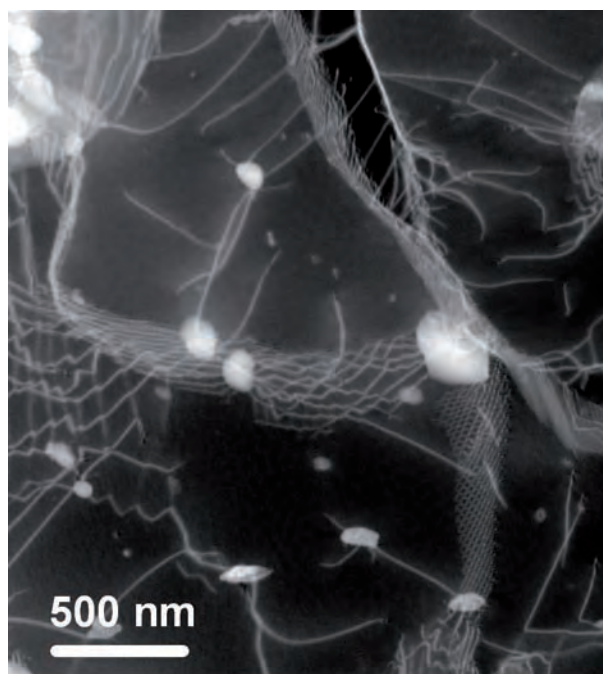
Fig. 4: *TEM micrograph (STEM HAADF) of dislocation particle interactions in a tempered martensite ferritic steel.*

Examples for the research output:

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INTER-DEPARTMENTAL RESEARCH ACTIVITIES – SELECTED HIGHLIGHTS

Fe-based Laves Phase Precipitates in High-Temperature Steels

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

An option to tailor the properties of steels or related Fe-based alloys for structural applications is the addition of transition metals. One of the frequently used essential alloying elements is Nb, which acts in a wide variety of materials for ambient and high temperature applications in multiple ways. Typical mechanisms include solid solution hardening, micro-carbides or carbo-nitrides, and the formation of intermetallic phases. Particularly the latter aspect has recently attracted increasing attention as alloys strengthened by fine precipitates (< 1 µm) of the Laves phase Fe_2Nb offer considerable strength and creep resistance at elevated temperatures [1].

A set of experiments with these Laves phases have revealed an extraordinary and hitherto not understood dependence of its mechanical properties on the chemical composition. Since a profound understanding of the structure, stability, and mechanical properties of the Laves phases is essential to control the material properties of the steels, experimental and theoretical investigations of the pure Laves phases Fe_2Nb and $(Fe,Al)_2Nb$ have been performed and the phase equilibria in the respective binary and ternary systems have been studied. The authors have undertaken this work in the framework of the inter-institutional research initiative "The Nature of Laves Phases" (s. p. 34) and the BMBF joint project "Ferrit950" [2-5].

It is noteworthy that a particular challenge of single-phase Laves phase material is its distinctly brittle behaviour even at elevated temperatures, which makes it difficult to produce defect-free samples that are large enough for mechanical testing. Therefore, a modified melting and casting route was developed for the production of bulk samples. It makes use of the levitation melting technique with in-situ heat treatment in a pre-heated crucible and slow cooling through the temperature range of the brittle-to-ductile transition [2]. Single-phase bars of 15 mm in diameter and at least 120 mm in length were obtained by this method allowing for example measurements of the Young's modulus as a function of temperature by the impulse excitation technique, Fig. 1.

In addition to the experiments, the Fe_2Nb Laves phase has been investigated by quantum-mechanical *ab initio* calculations. For this purpose the hexagonal
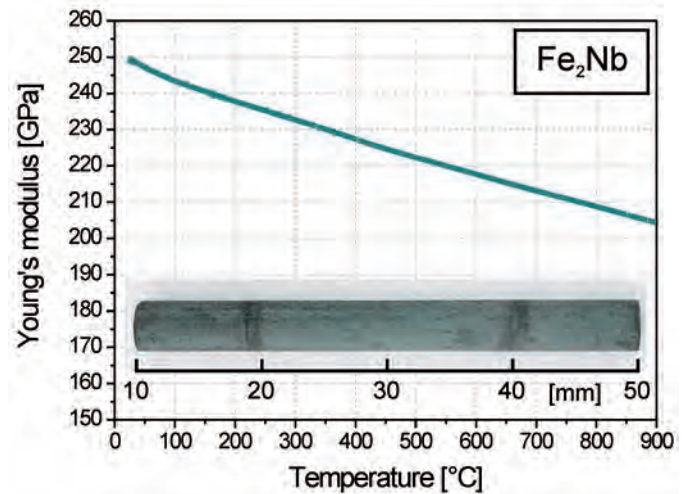

Fig. 1: *Dynamic Young's modulus of stoichiometric Fe_2Nb as a function of temperature. The photo shows the corresponding sample, which is a single-phase bar of 50 mm in length, after testing.*

crystal structure of the C14 structure type has been implemented, for which a degeneracy between two different antiferromagnetic structures has been identified, both of which were considered in the predictions. The stability analysis of this structure started with the determination of the single-crystalline elastic constants tensor C_{ij}, which gives direct insight into the directional dependence of the Young's modulus, Fig. 2. It reveals a rather strong elastic anisotropy (deviations from an ideal sphere), suggesting the use of a subsequent self-consistent crystal homogenization method to predict the polycrystalline Young's modulus at T = 0 K
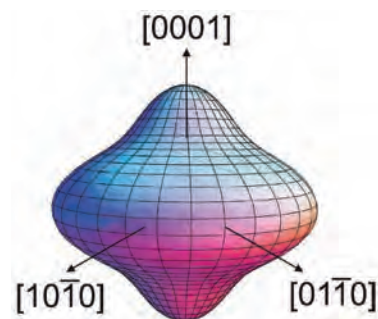

Fig. 2: *Quantum-mechanically calculated directional dependence of single-crystalline Young's modulus of Fe_2Nb with the hexagonal C14 structure. Shape deviations from an ideal sphere identify elastic anisotropy of the studied Laves phase compound.*
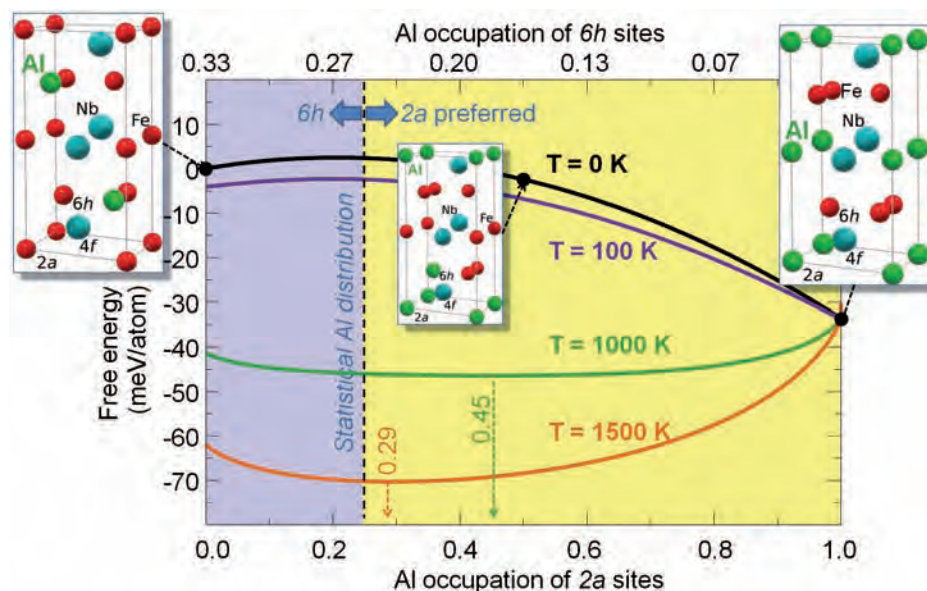
Fig. 3: *The ab initio calculated solution free enthalpies for $(Fe_{0.75}Al_{0.25})_2Nb$ at different temperatures. The black dots indicate results of ab intitio calculations, solid lines combine these results with a sublattice regular solution model. The values at the x axis at the bottom/top label the fraction of 2a/6h sites occupied by Al. The dashed line corresponds to a statistical distribution.*

also for cases where the grains do not assume a random orientation distribution (see also p. 133). The so derived value of 250 ± 22 GPa turned out to be in very good agreement with the experimental findings (the error bar is due to the above mentioned degeneracy).

However, as mentioned above, the mechanical properties vary strongly with composition. The yield strength drops to approximately half of its value on decreasing the Nb content from the stoichiometric value of 33.3 at.% to 30 at.%. This is a surprising result considering that the Fe_2Nb Laves phase of C14 type exists over a remarkably large composition range with Nb concentrations between about 25 and 37 at.% [3]. Furthermore, large amounts of Fe can be replaced by Al resulting in an extended two-phase field of the (α−Fe) solid solution with the Laves phase $(Fe,Al)_2Nb$ [4,5].

In a first step to understand how these chemical modifications affect the mechanical properties, the site preference of Al between the two Fe sublattices of the C14 structure has been studied, using again a combined experimental and theoretical approach. The Rietveld refinements of room-temperature XRD patterns of the ternary Laves phase show that – similar as in related C14 Laves phases like $(Cr,Al)_2Nb$ [6] and $(Co,Al)_2Nb$ [7] – Al prefers the 2a sites instead of the 6h sites.

In the *ab initio* investigation the site preference has been investigated at both low and elevated temperatures, making use of CALPHAD-like statistical sublattice models to determine the configurational entropy. The resulting free energies are shown for $(Fe_{0.75}Al_{0.25})_2Nb$ in Fig. 3 (considering a double-layer antiferromagnetic structure). Here, the

x axis at the bottom/top indicates the fraction of 2a/6h sites occupied by Al. As can be clearly seen, the 2a site has the lowest solution free enthalpy already at T = 0 K (pure *ab initio* data indicated by black dots). With increasing temperature, the larger number of sites and thus configurations in the 6h sublattice and the corresponding gain in configurational entropy, make the occupation of this sublattice more and more attractive. However, even for temperatures up to 1500 K the minimum of the free enthalpy curve is above x = 0.25 (the value corresponding to the statistical distribution), yielding a net-preference of the 2a sites.

The very promising agreement between theory and experiment provides a basis to systematically increase the complexity of these systems and to better understand how this affects the mechanical properties of Laves phases.

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Towards the Limits of Strength:
Pearlitic Nano-Compounds Studied at the Atomic Scale

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[3] Department of Materials Science and Engineering, Akita University, Japan

Heavily strained pearlite used in steel cords show more than 5 GPa tensile strength [1] and are among the strongest nano-structured bulk materials available today. Despite this great potential for engineering applications there exists a fundamental difficulty in correlating the enormous strength of this composite with its microstructural evolution upon severe plastic deformation. A refinement of the interlamellar spacing of the cementite phase is generally observed upon straining together with an increase in strength, which led to a description of this effect by the Hall-Petch relation. However, our recent study indicates that the Hall-Petch relation fails when the interlamellar spacing decreases to approximately 12 nm [2] after a true wire strain of $\varepsilon = 6.02$. The measured tensile strength of 6.5 GPa is far above the predicted value of 3 GPa by the Hall-Petch relation [3]. Thus, there must be additional reasons for the enormous strength. This may involve another important observation, namely, chemical (and potentially also structural) cementite decomposition upon straining. To elucidate this speculation, one has to understand the mechanism of cementite decomposition as well as the locations of the carbon atoms in ferrite on an atomic scale. Until recently it has been a great challenge to tackle this problem due to a lack of appropriate high-resolution characterization techniques. Owing to the availability of state-of-the-art atom probes, we are able to study cementite decomposition in pearlite in more detail.

The materials studied in this work are cold drawn commercial pearlitic steel wires of eutectoid (Fe-0.81C-0.49Mn-0.20Si wt. % or Fe-3.66C-0.48Mn-0.39Si at.%) and hypereutectoid (Fe-0.98C-0.31Mn-0.20Si-0.2Cr wt. % or Fe-4.40C-0.30Mn-0.39Si-0.21Cr at.%) compositions. A local electrode atom probe (LEAP 3000X HRTM, Cameca) was employed to analyze the carbon distribution in three dimensions. The instrument has several advantages over conventional atom probes such as larger probed volumes (~100 × 100 × 1000 nm^3) and a higher detection sensitivity due to an improved mass resolution ($\Delta m/m = 1/1100$, FWHM at 27 amu). Therefore, cementite decomposition can be studied with better statistics than in previous studies.

Fig. 1 shows that the tensile strength monotonically increases with true drawing strain up to $\varepsilon = 6.02$. In contrast, the corresponding carbon concentration in the ferrite saturates at $\varepsilon > 4$. The APT maps shown in Fig. 2 (next page) indicate a refinement of the
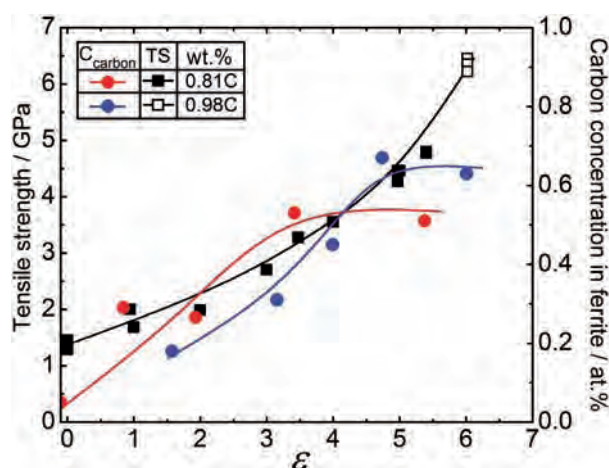

Fig. 1: *Tensile strength (TS) and carbon concentration (c_{carbon}) in ferrite as a function of true wire strain. Black symbols are for tensile strength. Red and blue symbols are the carbon concentrations in ferrite for pearlitic steel wires with eutectoid and hypereutectoid compositions, respectively.*

spacing of the cementite lamellae from 25 nm for $\varepsilon = 2$ to 13 nm for $\varepsilon = 5$, which is in good agreement with TEM observations. The maxima and minima shown in the 1D carbon concentration profiles (see Fig. 2b) represent the carbon concentrations in cementite and ferrite, respectively. We clearly observe a reduction of the carbon concentration in cementite and its enhancement in ferrite with increasing strain. It is worth noting that cementite does not completely dissolve even at $\varepsilon = 5$. The 3D carbon atom maps shown in Fig. 3a suggest that carbon atoms segregate at grain boundaries in ferrite. More data observed at different drawing strains indicate a heterogeneous distribution of carbon in ferrite (see Fig. 3b) which is supported by analyzing the distribution of the nearest neighbor distance of the carbon atoms.

Based on these findings we suggest that the decomposition of cementite is driven by the difference in the high binding energy of carbon at ferrite lattice dislocations (0.75 eV [4]) and the lower binding energy of carbon in cementite (0.4 ~ 0.42 eV [5]). Hence, dislocations can drag carbon atoms out of the cementite into the ferrite during deformation. It is well known that severe plastic deformation results in a nano-grained structure with a negligible density of free dislocations inside the grains. This may be confirmed in Fig. 3b where the carbon atoms are segregated mainly at the grain boundaries as well
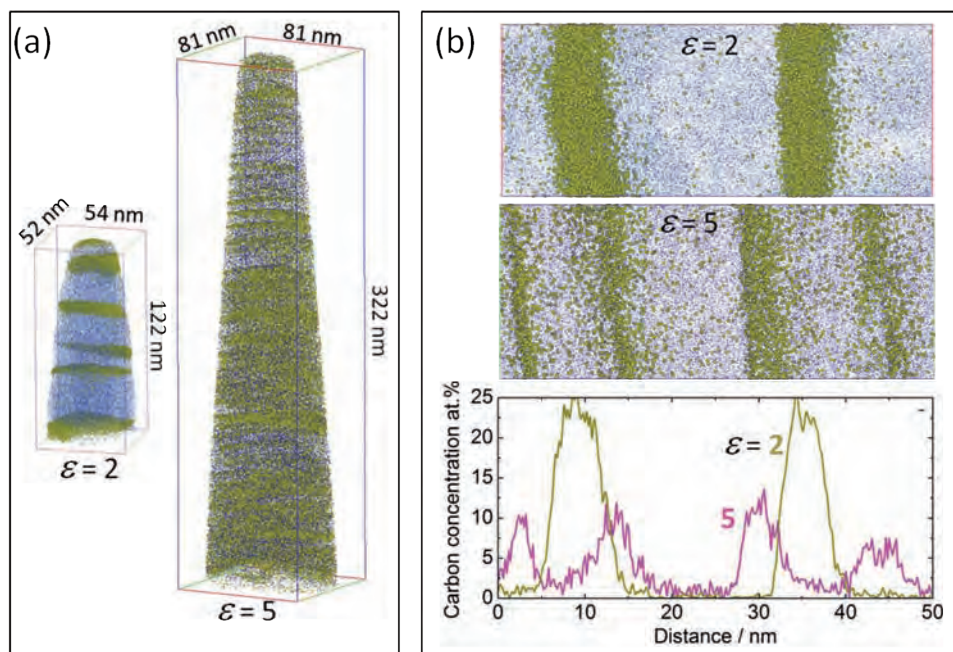
Fig. 2: *(a) 3D atomic maps of cold drawn wires for ε = 2 and 5. For clarity only 2% of iron (blue) and 20% of carbon (yellow) atoms are displayed. (b) Atom maps for the selected volume of 50 x 20 x 4 nm³ from (a) for ε = 2 (upper) and 5 (middle). 100% of the carbon and 50% of the iron atoms are shown. The bottom figure shows the corresponding 1D carbon concentration profiles along the direction perpendicular to the lamellar interfaces.*

as around a few individual dislocations. The pinning effects of the carbon atoms on dislocation glide and grain boundary motion leads to an increase in strength. The phenomenon that the tensile strength increases further with drawing strain whereas the carbon concentration in ferrite saturates (see Fig. 1) may be due to a further increase in the misorientation of the grain boundaries. This leads to additional strengthening as it impedes dislocation penetration and migration of grain boundaries. Beyond the elementary interaction between carbon atoms and lattice dislocations, we also consider a dislocation-shuffle mechanism to contribute to the deformation-enhanced decomposition of cementite, as discussed in [6].

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Fig. 3: *(a) Top: 3D carbon maps with an iso-concentration surface drawn at 7 at.% C for ε = 2. 50% of the carbon atoms are displayed. The two grain boundaries, GB1 and GB2, with carbon segregations, are marked by arrows. Bottom: Detailed carbon atom map for the selected volume (pink-colored box from top image) showing the cross section of GB2. (b) Distribution of the carbon atoms in ferrite of pearlitic wires with various strains. The volume of each box is given in Length x Height x Depth.*
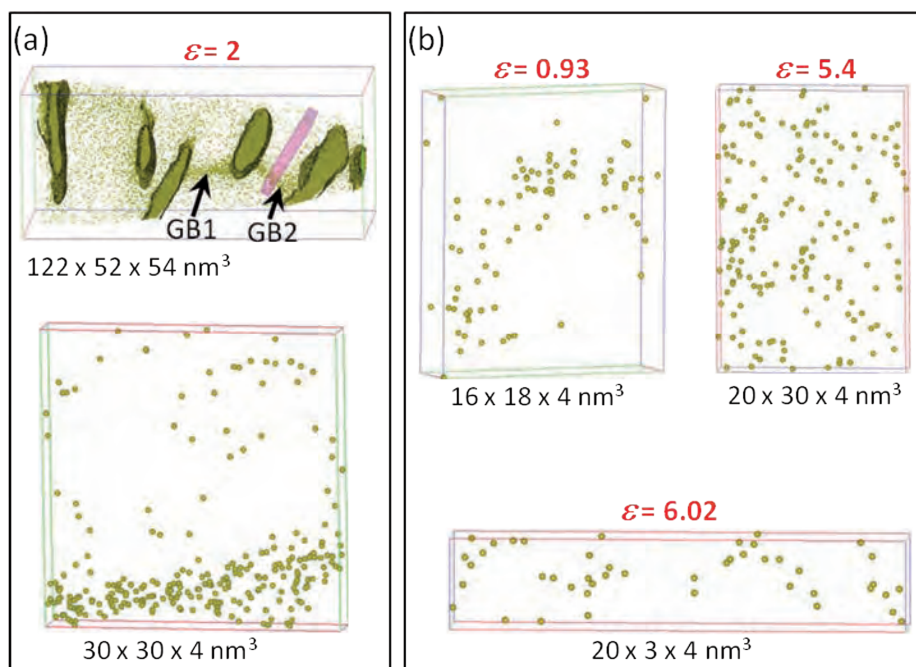
Structure and Corrosion of Iron-based Metallic Glasses during Crystallization

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Metallic glasses (MGs), often referred to as amorphous metals, lack long-range order and can be considered as frozen atomic configurations of a liquid phase [1]. The combination of metal properties with the formability of usual oxide glasses makes research on MGs very attractive both for fundamental understanding and for the development of tailored technological materials in metallurgy. The absence of microstructural features such as crystal plains, grain and phase boundaries or dislocations, contributes to their special properties [2-4]. Moreover, the properties of amorphous alloys also depend on their thermal history. Upon annealing, thermodynamically stable crystalline phases form from the metastable amorphous phase in a devitrification process. The nanocrystalline structure that nucleates and evolves after annealing changes the alloy corrosion resistance and other properties [5-7]. The control of introducing the respective grain boundaries and segregation profiles by temperature make these alloys also to an interesting model system for fundamental corrosion studies.

Among MGs, amorphous steels, i.e. Fe-based alloys, own valuable properties including excellent corrosion resistance, high specific strength, and probably the best thermal stability among metallic glasses [8-10]. The Fe-based alloy with the nominal $Fe_{50}Cr_{15}Mo_{14}C_{15}B_6$ composition has good mechanical properties and glass forming ability (GFA) [11]. In the present work, we investigate the changes in structure, local composition and corrosion behaviour of this alloy upon thermal history and crystallization state. The material was prepared by arc-melting a mixture of the constituents in a purified argon atmosphere. The resultant homogeneous alloys were melted again to prepare melt-spun ribbons of 50 μm thickness and 3 mm wide. For a number of samples crystallization was induced by thermal annealing of ribbons in an argon atmosphere. The samples were annealed at different temperatures (550-800º C), 20 minutes for each set temperature. These temperatures were selected according to the corresponding glass transition temperature T_g (544ºC), and crystallization temperatures T_{x1} (600ºC) and T_{x2} (623ºC) as a reference as determined by differential scanning calorimetry (DSC).
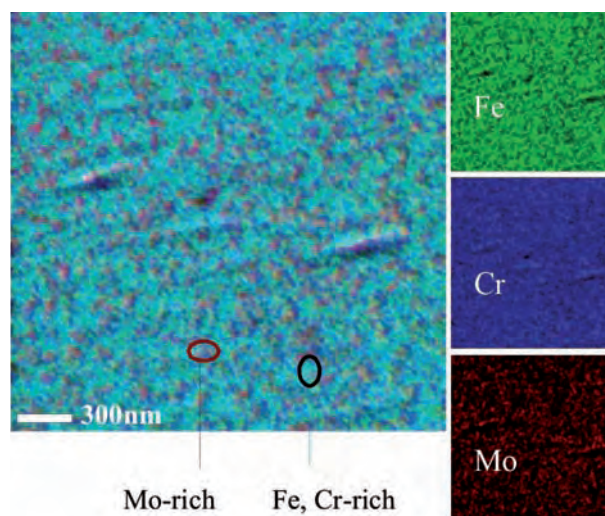

Fig. 1: *SAM map of fully crystallized MG $Fe_{50}Cr_{15}Mo_{14}C_{15}B_6$ (800°C, 20 min).*

X-ray diffractograms suggest that the main phases formed during crystallization are carbides and borides of the form $M_{23}(C,B)_6$, with M=Fe or Cr, with weaker additional signatures corresponding to a CrMo phase. Nanometer-sized crystallites were formed upon annealing, which renders high-resolution scanning Auger microscopy (SAM) and atom probe tomography (APT) essential techniques to understand the structural and compositional changes. Fig. 1 shows a SAM map of the fully-crystalline sample surface, annealed at 800ºC during 20 min, after removing a surface layer of 300 nm by sputtering. The surface shows 10-30 nm large Mo-rich inclusions in a Fe-Cr rich matrix. While SAM shows the chemical lateral composition of the surfaces evaluated in the corrosion tests with a resolution of below 10 nm, APT addresses the internal microstructure with an even better resolution. The combination of SAM and APT can thus link surface properties like corrosion behavior with unprecedented detail in morphology and composition. In agreement with the SAM result, Fig. 2a and b (next page) show APT data obtained from a fully-crystallized sample (800°C, 20 min). Mo-rich and Fe-Cr-rich areas are clearly visible. Boron and carbon segregate to FeCr / Mo interfaces.
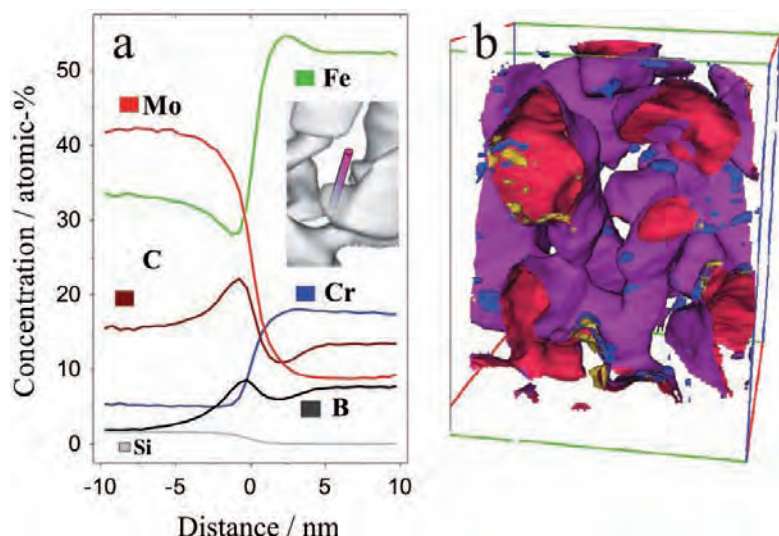
Fig. 2: *With near atomic-scale resolution, metallic glass is exposed (volume: 106 nm X 90 nm X 90 nm containing 23,885,434 atoms) via 3D-APT. Line analysis (a) and selected image (b) of interfaces and precipitates in fully-crystallized MG (800°C, 20 min). Higher concentrations of the minority C and B atoms are indicated with iso-concentration surfaces (yellow, blue) revealing their segregation between the Mo-rich (red) and FeCr-rich (purple) phases.*

Linear polarization tests in 0.1M HCl were performed to evaluate the corrosion behaviour. The corrosion tests show that fully amorphous steel presents a higher pitting or breakdown potential and a wider passive range than the partially and fully crystallized ones. The amorphous alloy exhibits hence a better corrosion resistance behaviour. After the corrosion attack the surfaces show pits as can be seen in the inset SEM of Fig. 3 for the fully nano-crystalline sample. The breakdown potential decreases considerably with crystallization and this loss in corrosion resistance can be attributed to the nanometer-scale phase separation in the heat treated material. But clearly the phases of different composition, including the grain boundaries, lead to a variation in the stability of the corresponding surface oxide scales as well as to a different proneness towards selective dissolution of the respective parts itself. The exact mechanisms are still evaluated.

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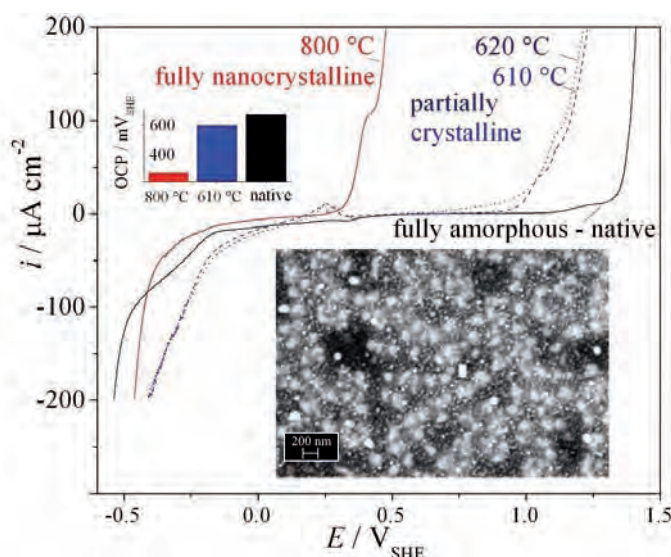11. Ponnambalam, V.; Poon, S.J.; Shiflet, G.J.: J. Mater. Res. 19 (2004) 1320.

Fig. 3: *Corrosion behaviour of as-produced amorphous MG, a fully-crystallized sample (800°C, 20 min), and an intermediate state (620°C, 20 min). E vs. Ag/AgCl. The inset shows an SEM image of a pitted surface (800°C, 20 min) after corrosion test.*

Gold Nanostructures Born from the Fe–Au Eutectoid

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The controllable preparation of nanocrystals with different shapes, exposed surfaces and assemblies is very important in terms of possible applications due to the anisotropic properties of crystals [1,2]. A novel approach, directional decomposition of an Fe–Au eutectoid alloy, to obtain Au nanostructures is presented in this work. During this process, the two alloying elements segregate and result in two pure phases. Directional solidification in combination with solid-state decomposition of an Fe–Au eutectoid alloy yields Au nanobelt arrays in the α-Fe matrix. Modifying the metallurgical procedures, i.e. directional solid-state decomposition without directional solidification, results in the formation of square-shaped Au nanoplates [3-5]. In both cases, the Au nanostructures exhibit a faceted morphology indicating the faceted nature of the Au phase. By nature of this method, the obtained materials are single crystalline [6,7].

An eutectoid Fe–Au pre-alloy with 2.3 at.% Au was prepared using 99.999% Au and 5 times zone refined Fe, by induction melting under an Ar atmosphere and drop casting into a cylindrical Cu mould [6]. After subsequent fitting into alumina crucibles, samples were directionally transformed in a Bridgman type solidification furnace with resistance heating. Afterwards, it was cut in $1\times1\times0.1$ cm^3 pieces and ground for further treatment.

A well controlled electrochemical treatment enables partial selective dissolution of the matrix, thus arrays of upstanding nanobelts of regular spacing can be obtained, as shown in Fig. 1a. Variation of the parameters of the electrochemical treatment gives precise control over the length of the exposed nanobelts. The length of the nanobelt arrays could be controlled from less than 200 nm to dozens of micrometers. Considering that the thickness of the nanobelts is only about 25-30 nm, the aspect ratio can reach more than 2000! By the nature of the method, as well as indicated by electron back scattering diffraction (EBSD), each nanobelt is single crystalline, as can be seen from Fig. 2. Moreover, the nanobelts are iso-oriented so that each nanobelt is a clone of it's neighbors.
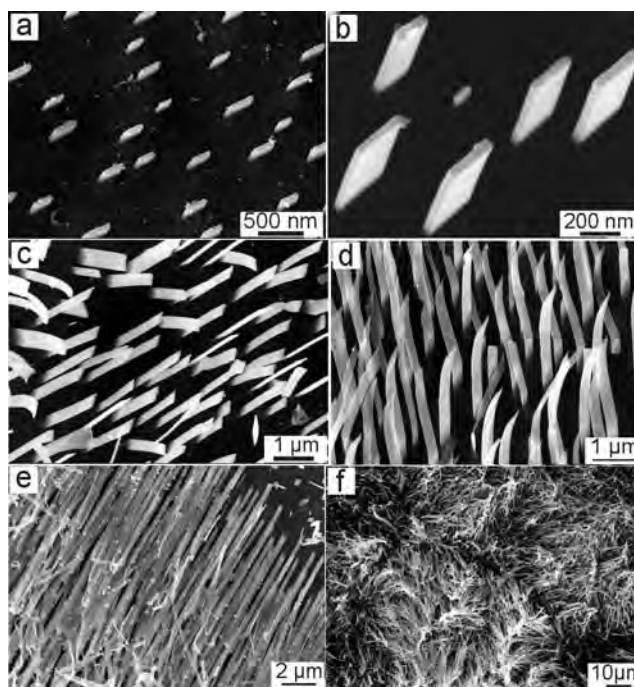

Fig. 1: *FE-SEM images of as-prepared Au nanobelt arrays with different exposed lengths (a, b) 250 nm, (c) 1 µm, (d) 2 µm, (e) 10 µm, and (f) 30 µm.*
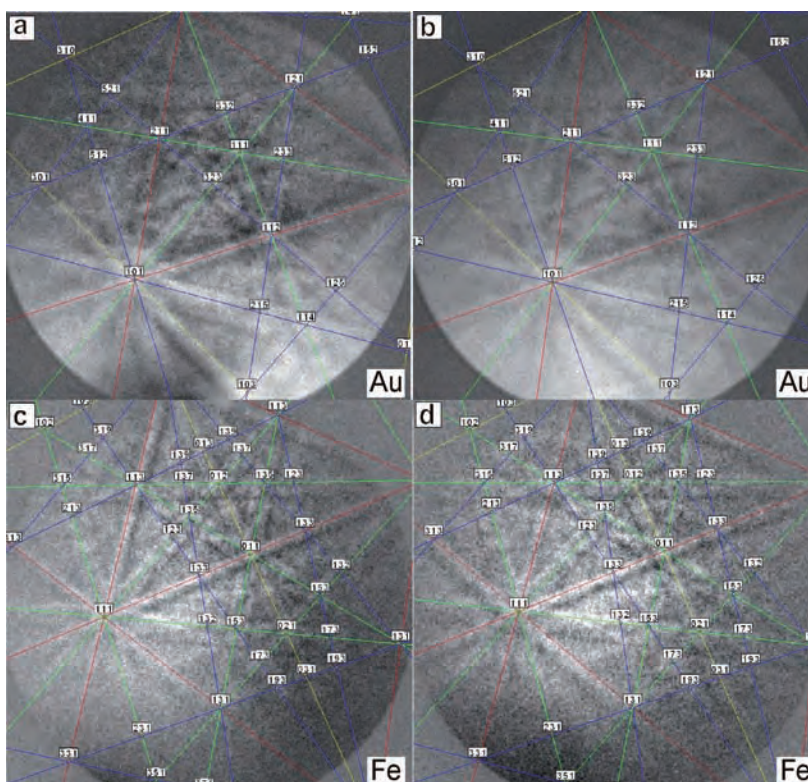

Fig. 2: *EBSD patterns of Au (a and b) and Fe (c and d) in one sample, which proved that gold nanobelts have the same crystallographic orientation.*
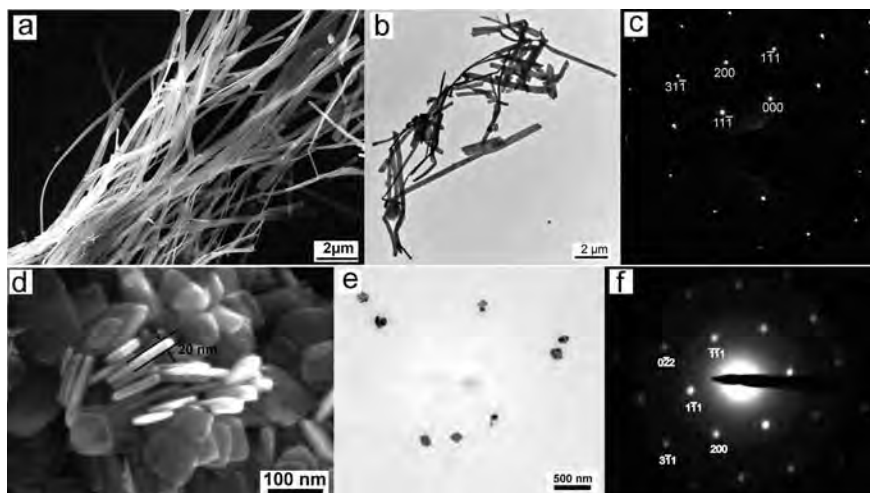
Fig. 3: *(a, d) FE-SEM, (b, e) TEM images of the free gold nanobelts or nanoplates; and (c, f) the corresponding SAED pattern of a single gold nanobelt or nanoplate, respectively.*

containing alkaline solution. This method is convenient, and more importantly, the surface structures of the samples are preserved. Afterwards, the superficial crystallographic structures of the Au nanobelts and nanoplates are characterized by means of underpotential deposition and cyclic voltammetry. These surface structure sensitive reactions further proved the dominance of {110} crystallographic surface for both samples, as shown in Fig. 4.

Also, free Au nanobelts or nanoplates can be obtained through complete iron matrix dissolution. This was achieved by a wet chemical method in the absence of any surfactant which leads to the formation of either free nanobelts or nanoplates. Fig. 3 shows the morphological and crystal characterization of the obtained nanobelts and nanoplates. The nanobelts can be more than 60 µm long, thus exhibiting extremely high aspect ratios. The nanoplates show a square shape with slightly truncated corners. Furthermore, from Fig. 3 c and f, one can see that both nanobelts and nanoplates are enclosed with unique {110} surface, which is much less common for fcc Au.

To further confirm the unique superficial features, underpotential deposition (UPD) of Pb and cyclic voltammograms (CV), both are very sensitive to the surface structure, were used to characterize the obtained nanostructures. However, before any electrochemical characterization, the surface of the nanostructure must be cleaned due to the high sensitivity of the electrochemical reactions. The surface was well cleaned by electrochemical deposition/dissolution of thin PbO_2 layers in a Pb^{2+}

In summary, for the first time, arrays of single crystalline gold nanobelts with long-range identical crystallographic orientation, free Au nanobelts and nanoplates with unique square shape were obtained through a directional solidification of an Fe–Au eutectoid followed by a phase selective etching process. The method is simple, convenient, economical, and easily applicable on a large scale. These unique properties allow a quantitative study of the spectroscopic properties as a function of the electrochemical potential and crystallographic orientation.

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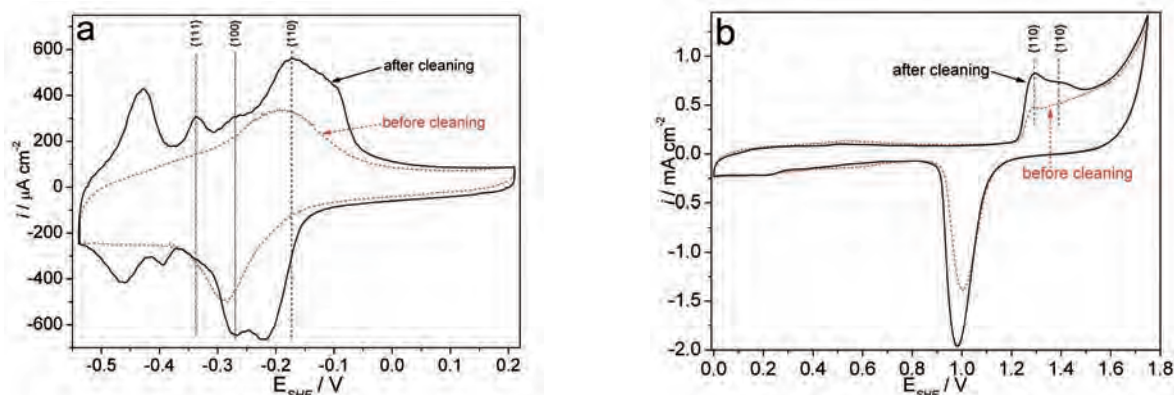
Fig. 4: *Cyclic Voltammograms (CVs) of Au nanobelts in (a) 0.1 M NaOH+10^{-3} M $Pb(NO_3)_2$, and (b) 0.01 M H_2SO_4 before and after the deposition/dissolution of PbO_2 film, respectively. Scan rate: 20 mV s^{-1}.*

Alloy Design Based on Combining First-Principles and TEM Methods

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Pure magnesium and most commercial wrought magnesium alloys exhibit a low room temperature ductility which can be significantly increased by the addition of rare earth elements in solid solution (Fig. 1). Understanding the mechanisms causing this ductility enhancement on an atomistic and electronic-structure level would provide a systematic approach to identify further favourable alloying elements. We have therefore performed complementary investigations by experimental and *ab initio* methods.

Mechanical testing of pure Mg and a single-phase solid solution Mg–3 wt.% Y alloy showed that the addition of yttrium increases the room temperature ductility about 5 times and leads to a well-balanced work-hardening during deformation [1-2].

The main deformation modes in pure Mg are limited to basal <a> dislocation slip and $\{10\bar{1}2\}<10\bar{1}1>$ tensile twinning. Consequently, the strain is localized in few shear bands and crack formation starts early. Contrarily, in the Mg-Y alloy additionally $\{10\bar{1}1\}<10\bar{1}2>$ compression twinning, $\{10\bar{1}1\}\{10\bar{1}2\}$ secondary twinning and pyramidal <c+a> dislocation slip are frequently observed [1,2]. In particular, the activity of <c+a> slip systems enables interaction of different slip systems resulting in a homogeneous deformation [1,2]. As grain refinement, precipitation hardening, shear banding, decreased c/a ratio, and changed Peierls potentials cannot be responsible for the higher activity of compression, secondary twinning and <c+a> dislocation slip [2], it is commonly assumed, that the addition of yttrium changes the stacking fault energies (SFE). A modified SFE would also affect the critical resolved shear stresses (CRSS) associated with the competing shear mechanisms and, hence, would influence their relative contributions to the overall deformation.

In principle, three basal stacking faults can form in hcp magnesium: two intrinsic faults I_1 (stacking sequence …ABABCBCBC…) and I_2 (…ABCACAC…) and an extrinsic fault E (…ABABCABAB…). Previous and our own density functional theory (DFT) calculations of these stacking faults in pure Mg [3] showed that E is energetically unfavourable. For both, I_1 and I_2, relatively high stacking fault energies (20-50 mJ·m^{-2}) resulting in an equilibrium distance of the partials below 1.27-1.67 nm were obtained [3].

TEM observations on slightly (1.5 % engineering strain) cold deformed pure Mg and Mg–3Y reveal a high density of stacking faults in the Mg–Y alloy, while in the pure Mg stacking faults were observed only inside twins.
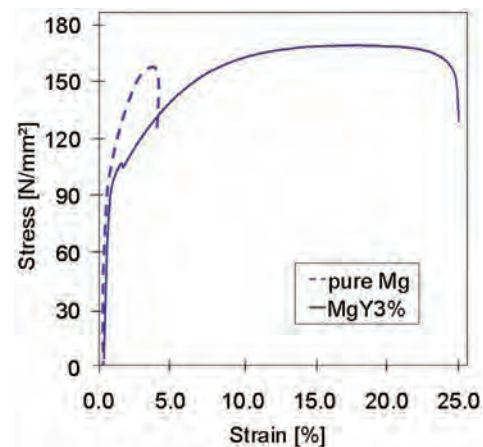
Fig. 1: *Stress-strain curves of tensile test results obtained at room temperature for pure Mg and Mg–3 wt.% Y.*

Detailed Burgers vector (b) and displacement vector (R) analysis according to the g*b resp. g*R visibility criterion of these stacking faults was performed and is exemplary shown in Fig. 2 (next page). From the analysis it can be concluded that both intrinsic stacking faults are formed in Mg–3Y. The corresponding stacking fault energies are calculated based on the dissociation width of the partial dislocations according to the equation

$$\gamma = \frac{Gb^2}{8\pi d} \frac{2-v}{1-v}\left(1 - \frac{2v}{2-v}\cos 2\beta\right)$$

Here, γ is the stacking fault energy, G the shear modulus, v the Poisson`s ratio, b the Burgers vector of the partials, β the angle between the partials, and d the splitting width of the partials.

In the case of I_1 (Fig. 2(a)) the average splitting of the partials is 40-80 nm, which corresponds to an I_1 stacking fault energy of 0.482-0.964 mJ·m^{-2}. For I_2 (Fig. 2(b)) the stacking fault energy amounts to 0.964-1.964 mJ·m^{-2} with an average dissociation width of 20-40 nm.

In order to obtain a deeper insight into the mechanisms responsible for the increased ductility observed in the Mg-Y alloys, the above described experimental studies have been complemented by a quantum-mechanical study of the compositional dependence of intrinsic stacking fault (ISF) energies. Employing DFT calculations, the ISF energies have been determined within the axial next-nearest-neighbour Ising (ANNNI) model [4], which has already been successfully applied to austenitic stainless steels [5] and Fe-Mn alloys [6].

The ANNNI model provides a reasonable energetic description of the faulted crystal. It uses as input a few

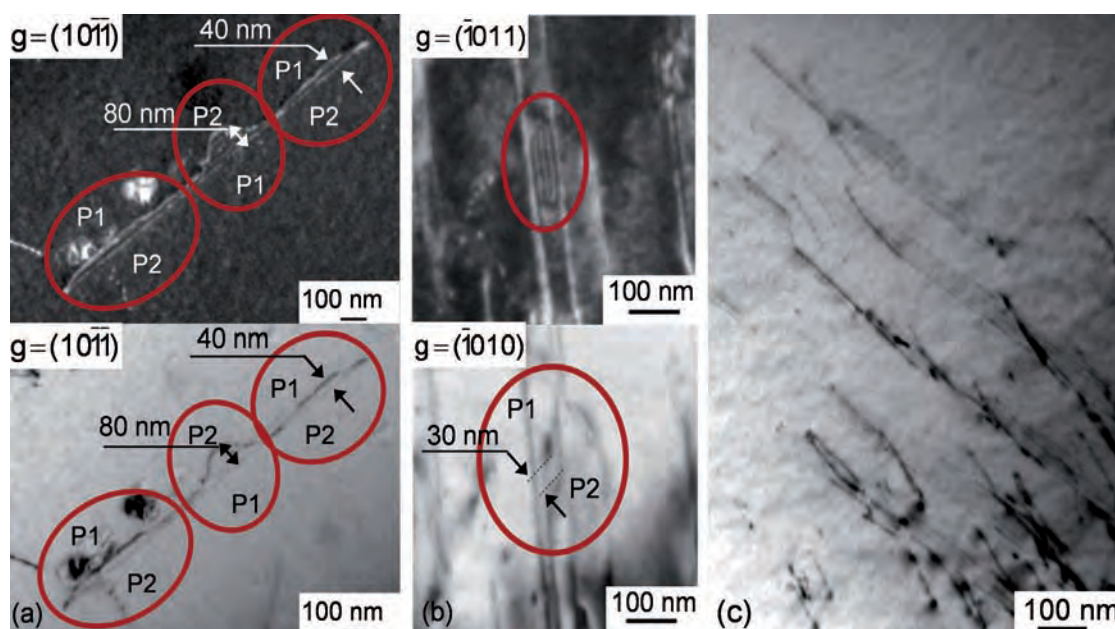**Fig. 2:** *Stacking faults in 1.5 % cold deformed Mg-3Y: (a) the intrinsic stacking fault I_1, (b) the intrinsic stacking fault I_2 and (c) after 5 % cold deformation; P1 and P2 are the partial dislocations bounding the stacking faults.*

simple structures with different stacking sequences (Fig. 3). This allows to avoid explicit DFT calculations of the stacking faults, and to focus instead on computationally efficient supercells containing only a moderate set of atoms. The energies of the stacking faults I_1, I_2, and E are computed considering the energies of the fcc (ABCABC stacking), hcp (ABAB stacking), and double-hcp (ABACABAC) sequences.

The resulting intrinsic stacking fault energies of Mg-Y alloys possess a strong non-linear compositional dependence: Despite the fact that pure yttrium has higher ISF energies than pure Mg for both basal-plane stacking faults I_1 and I_2, small additions of yttrium into Mg (exactly $Mg_{15}Y$ and $Mg_{14}Y_2$) result in a significant reduction of the I_1 intrinsic stacking fault energy in excellent agreement with experimental data.

From a phenomenological point of view the ductility increase is related to higher activities of compression,

Fig. 3: *Schematic representation of the ideal hcp and intrinsic stacking fault geometries.*

secondary twinning and <c+a> dislocation slip in Mg-Y alloys. These higher shear activities can be easily explained by the significantly decreased stacking fault energy through the addition of Y. At the same time a lower basal stacking fault energy causes a less mobile basal dislocation substructure so that <c+a> slip can yield a higher shear contribution.

An in-depth analysis of the theoretical data shows that the reduced ISF energy is a direct consequence of the dramatically reduced thermodynamic stability of hexagonal Mg–Y solid solution when the yttrium concentration approaches its solubility limit in Mg. The deduced lowering of the thermodynamic stability is supported by the Mg–Y phase diagram where for yet higher concentrations of Y in Mg two-phase alloys containing $Mg_{24}Y_5$ cubic-structure precipitates are formed.

In conclusion, combining *ab initio* with advanced experimental dislocation characterization approaches provides an efficient and accurate toolset to determine and understand critical microstructure parameters as needed for materials design of complex structural engineering materials.

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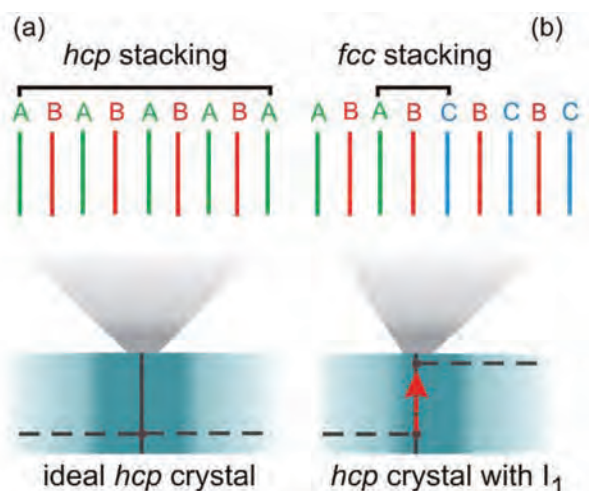6. Dick, A.; Hickel, T.; Neugebauer, J.: Steel Res. Int. 80 (2009) 603.

Early Stages of Precipitation Nucleation in Electrical Steels Studied by Atom Probe Tomography and Kinetic Monte Carlo Simulations Based on DFT

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Electrical steels play an essential role in the generation, transformation, distribution, and use of electrical power and belong to the most important soft magnetic materials produced today. One of the currently intensively discussed applications is the use of electrical steel sheets in engines for electrical cars. The soft magnetic properties are relevant for the cyclic magnetization in the electric engine.

The magnetic behavior of these materials is largely determined by the microstructure: In particular, a ferritic coarse grain structure, as used in standard soft magnetic steels with 3 wt. % of silicon, allows an unhindered movement of Bloch walls, leading to the desired magnetic properties. As this microstructure implies relatively weak mechanical properties, the existing electrical steels cannot be used in mechanically highly stressed parts of the electrical motor. In this context we study the precipitation of a second phase in order to achieve a strength enhancement in electrical steels.

It is well known that due to the low solubility of copper in bcc iron-silicon, the addition of a few percent copper leads to the formation of nanoscaled precipitates [1-3]. In our work, finely dispersed copper nanoparticles were produced by an aging treatment of a Fe-Si-Cu alloy (Si 3 wt.%, Cu 1 and 2 wt.%, respectively). Subsequently, 3D atomic scale chemical analyses were performed by using atom probe tomography (APT, LEAP 3000X HR) on both alloys aged at 450°C for 120 and 6000 min, respectively. APT was performed at a sample temperature of 60 K by a laser pulse energy of 0.4 nJ.

Fig. 1 shows the resulting 3D distribution of the Cu-rich clusters for different compositions and aging times in terms of iso-concentration surfaces plotted at 11 at.% Cu. The quantitative results are summarized in Table 1. They reveal that the cluster size as well as the mean Cu content inside them increases with aging time, reducing the solved Cu in the matrix. However, even after 6000 min aging time, we found a relatively high Fe content of up to 52 at.% within the clusters.

In order to understand these kinetic processes better we analyzed the APT data with respect to the early stages of cluster formation and precipitation in this system. Even during the growth and coarsening stages, ongoing nucleation of new atomic clusters was observed. For example in the 2 wt.% Cu-alloy aged for 6000 min, we observed parallel to the formation of precipitates with a mean size of about 6 nm, also clusters smaller than 1 nm, Fig. 2a (next page). This phenomenon leads to a bimodal cluster size distribution with two mean particles sizes, one at $d_1 = 1.1$ nm and a second one at $d_2 = 5.8$ nm, Fig. 2b.

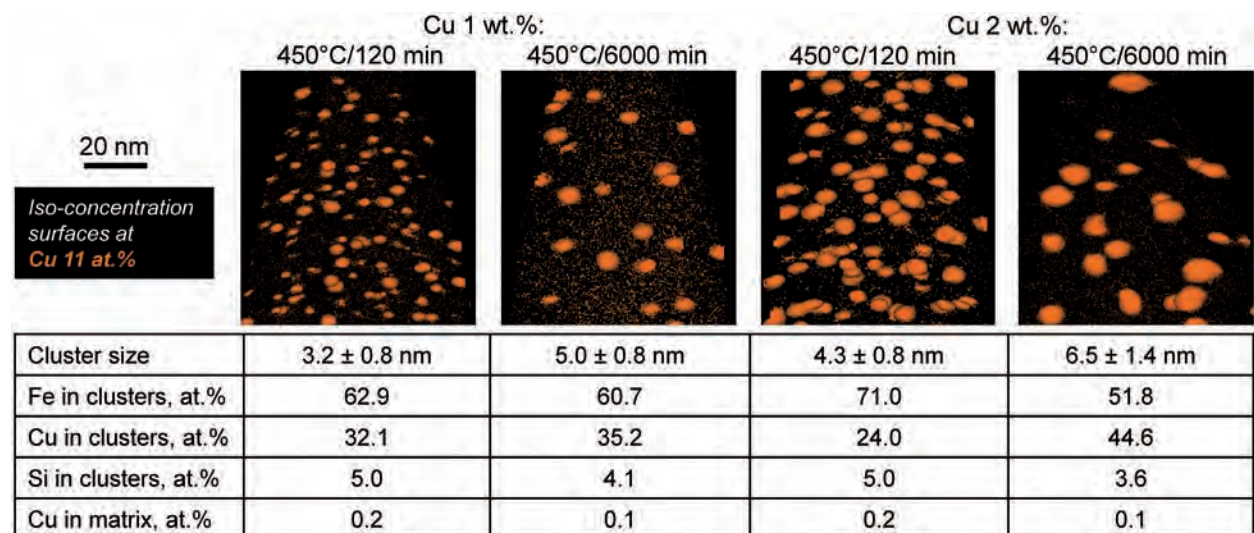|	Cu 1 wt.%: 450°C/120 min	Cu 1 wt.%: 450°C/6000 min	Cu 2 wt.%: 450°C/120 min	Cu 2 wt.%: 450°C/6000 min
Cluster size	3.2 ± 0.8 nm	5.0 ± 0.8 nm	4.3 ± 0.8 nm	6.5 ± 1.4 nm
Fe in clusters, at.%	62.9	60.7	71.0	51.8
Cu in clusters, at.%	32.1	35.2	24.0	44.6
Si in clusters, at.%	5.0	4.1	5.0	3.6
Cu in matrix, at.%	0.2	0.1	0.2	0.1

Fig. 1: *APT results represented as 3D iso-concentration surfaces plotted at 11 at.% Cu for different samples. Table summarizes the quantitative analysis from APT analysis.*
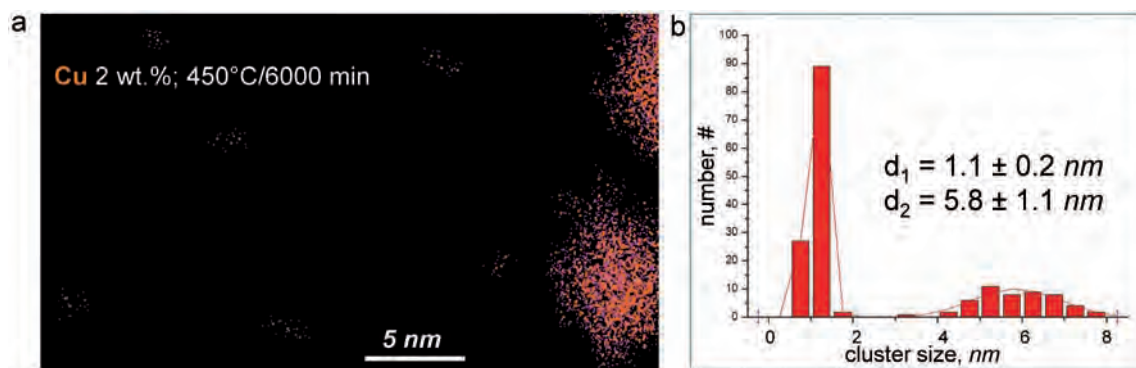
Fig. 2: *(a) Zoom into the 3D distribution of the Cu and Fe atoms obtained from the cluster search analysis of the aged 2 wt.% Cu-alloy (450°C, 6000 min). Beside the nm-sized precipitates, also clusters of less than 20 atoms were found. (b) Size distribution of the found cluster ensemble exhibits a bimodal character with two mean cluster sizes, namely, d_1 = 1.1 nm and d_2 = 5.8 nm.*

For analyzing the atomistic mechanisms behind the complex precipitation processes, kinetic Monte Carlo (kMC) simulations are being conducted on the ternary Fe-Cu-Si system. For this purpose, a kMC code has been developed, which has the flexibility to consider several atomic species and lattices including also e.g. grain boundaries. Atoms on the lattice can move via vacancy mediated jumps. The corresponding rates are determined using *ab initio* calculations in combination with harmonic transition state theory.

The *ab initio* calculations to obtain an accurate set of energies for the diffusion and interaction (binding) with other atoms have been performed using density functional theory (DFT) and the generalized gradient approximation for the exchange-correlation functional. Already these data revealed interesting insights: For example, two Si atoms within the bcc Fe matrix have a repulsive nearest neighbor interaction energy of 0.4 eV, while two Cu atoms have an attractive interaction of −0.3 eV. These results immediately explain why in the APT observations only Cu clusters are observed. The large repulsion energy between Si atoms is the reason why no Si accumulation in the clusters occurs, despite the fact that Si and Cu atoms are slightly attractive with a −0.1 eV interaction energy.

To gain some first qualitative understanding of the precipitation kinetics, initial calculations have been performed assuming renormalized effective jumping rates of the atoms without explicitly taking into account vacancies, Fig. 3. Using this model we could e.g. show that the size of precipitate clusters correlates with the annealing temperatures and inversely with the impurity interaction energies. This observation is in contrast to an intuitive estimate which might assume that an increased attractive binding energy between impurities will result in larger precipitates.

In conclusion, combining the experimental APT technique with *ab initio* based atomistic kMC simulations provides a powerful basis to understand and eventually control self-organized nucleation and coarsening of coherent nano-precipitates in a wide range of materials. Already first results obtained on the Fe-Si-Cu system are very encouraging and we see a high potential in continuing this approach.

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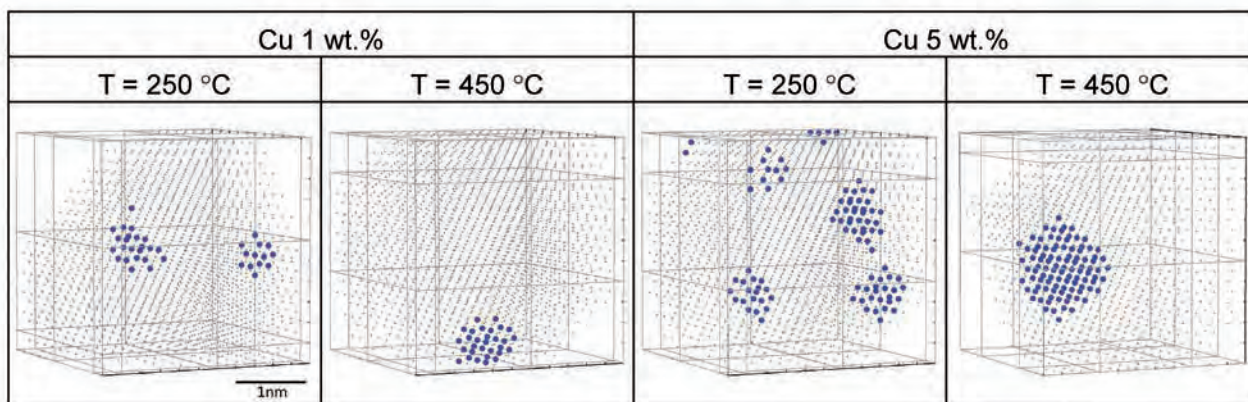
Fig. 3: *Close-up of the simulation cells of kinetic Monte-Carlo simulations for the precipitation of Cu (blue dots) in bcc Fe (lattice sites indicated with grey dots) based on effective jump rates. Two different concentrations and temperatures were used.*

Chemical Partitioning across Phase Boundaries in High-Strength Steel Studied by Atom Probe Tomography and Simulation

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Maraging TRIP steels combine precipitation hardening of martensite by intermetallic phases (maraging) with a TRIP effect, providing high strength and ductility simultaneously [1-4]. Important for improving ductility through the TRIP effect is not only the retained austenite after quenching but also the reverted austenite formed during aging. This reversion effect was investigated by EBSD, TEM, XRD and APT (atom probe tomography).

The investigated maraging TRIP steel with a composition of 12.2 % Mn, 1.9 % Ni, 0.6 % Mo, 1.2 % Ti, 0.1 % Si, 0.3 % Al, and 0.05 % C (at.%) was melted in a vacuum induction furnace. After solution treatment (1050°C/0.5 h) and water quenching the microstructure comprises martensite and 4-6 vol.% retained austenite. After aging (450°C/48 h) the austenite content increased to 15-20 vol.%, and the martensite matrix is decorated by homogeneously dispersed nanoscaled precipitations enriched in Ni, Al and Mn [1-4], Fig. 1. According to Thermo-Calc predictions an austenite content of about 40% is expected for equilibrium at 450°C.

Fig. 2 (next page) gives a local overview of the distribution of Mn atoms (blue) of an APT data set. Mn iso-concentration surfaces at 18 % are shown in yellow. Martensite regions are decorated by precipitates. In the center a region with retained austenite is visible which is indicated by the lack of precipitations and a Mn content of 12.2 %Mn, corresponding to the nominal composition.

Quantitative chemical analysis of the interfaces between austenite and martensite was performed using 1D concentration profiles computed over the region of interest (cylindrical units), Fig. 2a. We calculated the Mn content averaged over the 0.5 nm thick cross sections of the cylinders. For both interfaces, a strong increase in the Mn content up to 27 % was observed, Fig. 2b. Away from the interface, the content of Mn within the austenite amounts to about 12 % which is close to the average chemical composition of the alloy. Within the bulk martensite the Mn content amounts to about 10 %. Mn depletion in the martensite down to 6 % was observed close to the interface.

To verify the assumption that during aging the austenite/ martensite interfaces are moving towards the martensite (austenite growth), diffusion simulations using DICTRA were performed. The conditions at the moving interface are determined by the local equilibrium assumption, i.e. the chemical potentials of all diffusing elements assume

Fig. 1: *Microstructure of the maraging-TRIP steel after quenching and aging (48 hours / 450 °C). The upper EBSD image shows cubic martensite in green and retained austenite red. The TEM image shows precipitate-containing martensite and precipitate-free austenite. The bottom image is an APT reconstruction of martensitic and austenitic zones. Ni atoms are in cyan and Mn atoms in blue. The yellow iso-surfaces indicate 18 at.% Mn. The images reveal the hierarchy of the microstructure but the individual images were not exactly taken at the positions indicated.*
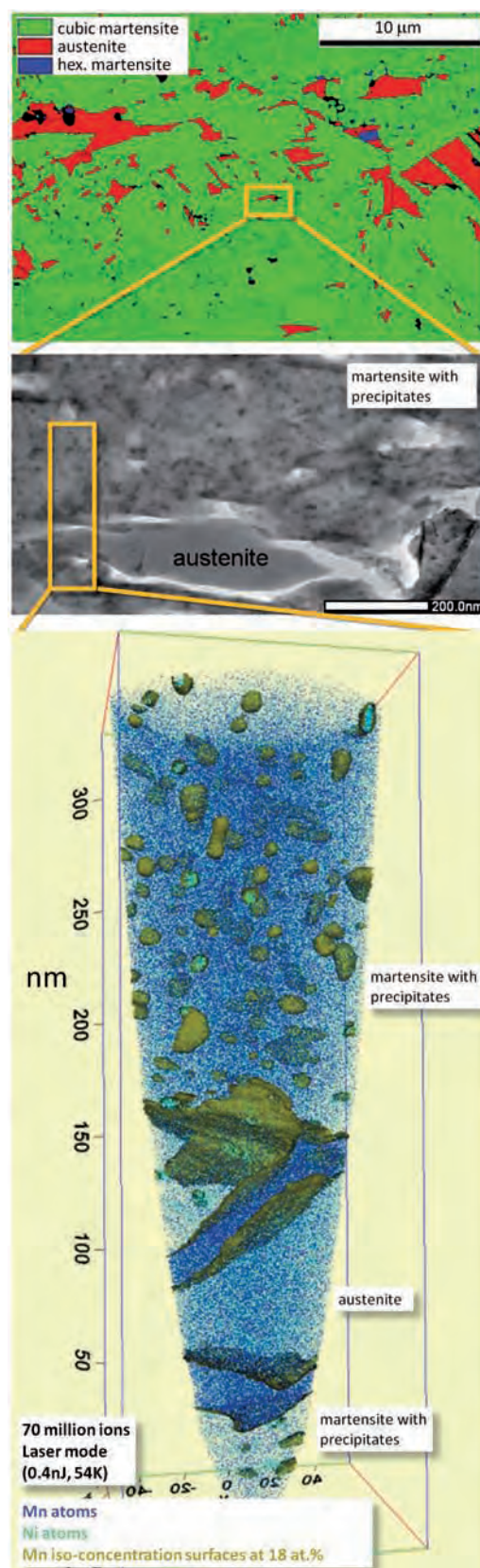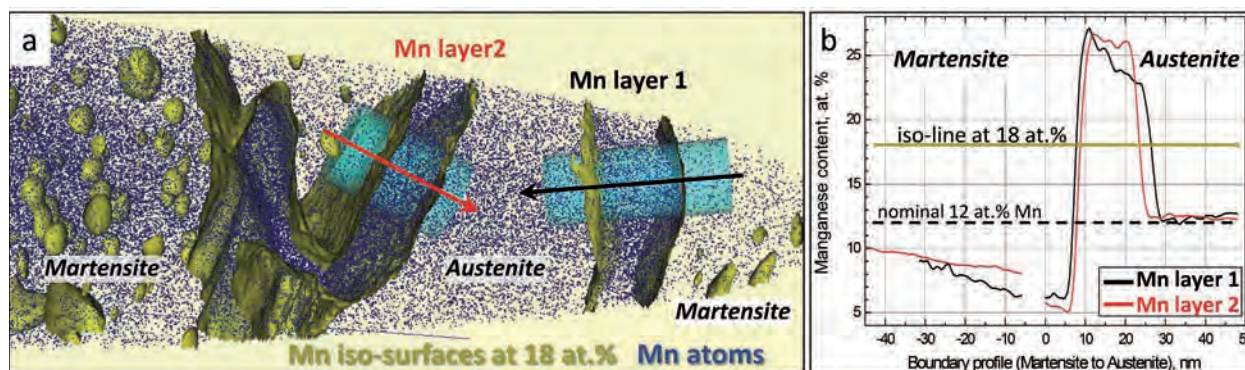
Fig. 2: *Quantitative chemical analysis of the interface regions between martensite and austenite (APT results): a) Atomic map section showing both phase boundaries. Iso-concentration surfaces for the distribution of Mn atoms (blue) were plotted at 18 at.% (yellow). 1D profiles along the cylindrical units (cyan) provide gradients of elements across the phase boundaries; b) Gradients in the Mn-content across the phase boundaries.*

the same value in ferrite and austenite. The value of the potentials is controlled by the mass balance condition. Diffusion of Mn, Mo, Ni, Si, and Ti atoms was considered in the calculation. The simulation was performed for the aging temperature 450°C.

The predicted composition profile of Mn between ferrite (cubic martensite) and austenite after an annealing time of 50h at 450°C is presented in Fig. 3. It indeed reveals that the interface has moved towards the ferrite side leaving behind an austenite layer with drastically changed composition. This prediction is in excellent agreement with the experimental results in Fig. 2b. This applies for the depletion profile of Mn in the martensite and also for the Mn-enriched interface zone.

We estimated the mean diffusion paths of Mn atoms in both phases using the diffusion coefficients obtained for 450°C. The diffusion constant of Mn atoms in a BCC iron matrix (ferrite) was $D_{BCC} = 1.75 \times 10^{-22}$ m^2/s and in the FCC iron matrix $D_{FCC} = 5.86 \times 10^{-24}$ m^2/s. The mean diffusion path λ of Mn atoms for an aging time of t = 48h was calculated using the volume diffusion equation for cubic metals: $\lambda = (6tD)^{1/2}$. In the BCC lattice it was about 13 nm and in the FCC lattice about 2.5 nm. Thus, the diffusion length of Mn in BCC is significantly larger than in

the FCC lattice. To take into account the high defect density of martensite (e.g. pipe diffusion), the mobility of the atoms in ferrite was increased by a factor of 45. For this case, the mean diffusion path of Mn in ferrite (which can be then treated as martensite) increases from 13 nm to about 90 nm.

The global equilibrium calculated with Thermo-Calc for 450°C predicts a high amount of Mn in austenite (27.6 at.%) and a low value (3 at.%) in ferrite. Hence, during aging a redistribution of Mn is expected. However, the global equilibrium only indicates the long term trends. The actual situation at the phase boundary is controlled by a local equilibrium.

The local boundary condition at the interface leads to the diffusion of Mn in martensite towards austenite. The chemical gradients of Mn predicted by DICTRA at the phase boundary revealed a good quantitative correlation to the experimental findings. The diffusion behavior of other alloying elements such as Ni, Ti, and Mo could also be reproduced in the dynamic simulation.

The partitioning at the martensite/austenite inter-face leads to the formation and growth of a new austenite layer on the existing retained austenite with drastically changed composition compared to the bulk. Such a layer will have an effect on the mechanical properties. This layer is likely to be one of the microstructural changes that is responsible for the increase in ductility during aging [1]. The other contribution for increasing the ductility stems from the tempering of the martensite during aging and was reported elsewhere [3].
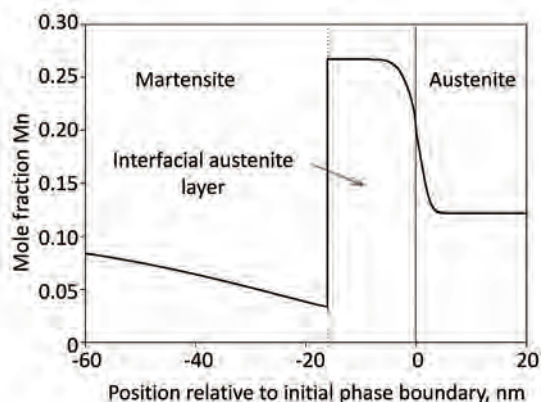
Fig. 3: *DICTRA calculation of Mn distribution at the mar-tensite/austenite interface. Martensite is treated as ferrite, but the mobility of the elements is increased by a factor of 45. The calculation assumed 450°C. The result is shown for the time step 180000 sec (50 h).*

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Defect Observation by Electron Channelling Contrast Imaging (ECCI) under Controlled Diffraction Conditions in the Scanning Electron Microscope

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The observation of specimens in the scanning electron microscope (SEM) by means of backscattered electrons (BSE) is a known technique that allows, in principle, observation of crystalline defects (grain boundaries, dislocations, twins) [1-3]. The method is also referred to as electron channelling contrast imaging (ECCI). It is based on the fact that the electron backscattering yield obtained from a crystal depends strongly on the incidence direction of the primary beam with respect to the crystal lattice planes. If the incidence direction is very close to the Bragg angle of some low-indexed set of lattice planes the backscattered intensity is very low because the primary electrons deeply channel into the lattice. As a result, in a microstructure image obtained with a BSE detector such areas appear dark. In contrast, if the incidence angle is out of the Bragg angle intensive backscattering occurs and such areas appear bright. Fig. 1a describes this relationship schematically. The described behaviour can be exploited to observe dislocations and other lattice defects as shown in Fig.1b: the area of interest is tilted such that a low-indexed set of lattice planes is excited in "two beam conditions", i.e. that the primary beam observes the Bragg angle with only this set of planes. This area then appears dark in the image. At dislocations the lattice planes are slightly bent out of the Bragg angle, resulting in a significant increase of intensity at these locations. Individual dislocations therefore appear as white lines on a dark background.

Until recently the ECCI technique was either done in an uncontrolled manner, where one hoped to obtain good observation conditions by just tilting the sample by few degrees [4,5], or by the use of electron channelling patterns (ECP) which allow direct selection of two-beam conditions [6]. ECP, however, have significant limitations, in particular low spatial resolution, fading on deformed material and unavailability on most modern SEM. In order to overcome these limitations we replaced the use of ECP by a combination of orientation determination by electron backscatter diffraction (EBSD) patterns and a simulation of ECP patterns from the determined orientation using dedicated software [7,8]. Crystal orientation determination by EBSD is performed at a high sample tilt angle in the order of 70 degree. Subsequently, the sample is tilted back to horizontal position and the ECP simulation software [9] is used
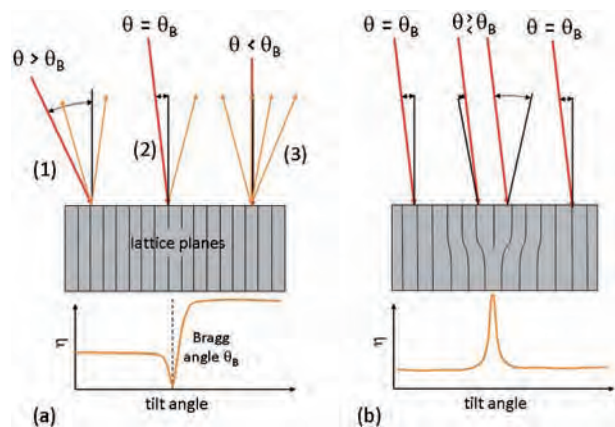
Fig. 1: *Schematic description of contrast formation in ECCI. (a) Dependence of backscattering yield η on the incidence angle θ of the primary beam with respect to a set of lattice planes with Bragg angle θ_B. (1) $\theta > \theta_B$: average back scattering; (2) $\theta = \theta_B$: strong channelling, weak back scattering; (3) $\theta < \theta_B$: strong back scattering; (b) Contrast behaviour at a dislocation under the conditions that the crystal lattice is illuminated at the Bragg angle.*

to determine the sample tilt and rotation angles required to obtain two-beam conditions. Finally the sample is rotated and tilted to the determined values and the image is recorded. In this way high contrast images can be obtained under controlled diffraction conditions in very short time. In Figs. 2 a and b (next page) example images obtained from a TWIP steel are shown. Here three different sorts of lattice defects are visible: Dislocations (1) are characterized by their curved line-shape appearance. Stacking faults (SF) (2) are usually limited by a sharp and straight edge on one side – which corresponds to the intersection of the fault plane with the sample surface. The opposite side continuously fades away because the distance between fault plane and surface increases continuously. Under certain circumstances, the partial dislocations which limit the SFs on the short sides are visible as well. Finally, fine twins (3) are visible. Twins can be distinguished from stacking faults by the fact that both limiting edges appear sharp.

The maximum contrast available in ECCI depends on the strength of backscattering which increases with increasing atomic number and density. Good dislocation contrast, however, can already be observed on magnesium with an atomic number of 12. The resolution of the technique can be assessed from

Fig. 2: *ECC images of various lattice defects in a deformed TWIP steel. The insets display the simulated electron channelling patterns for the particular imaging cond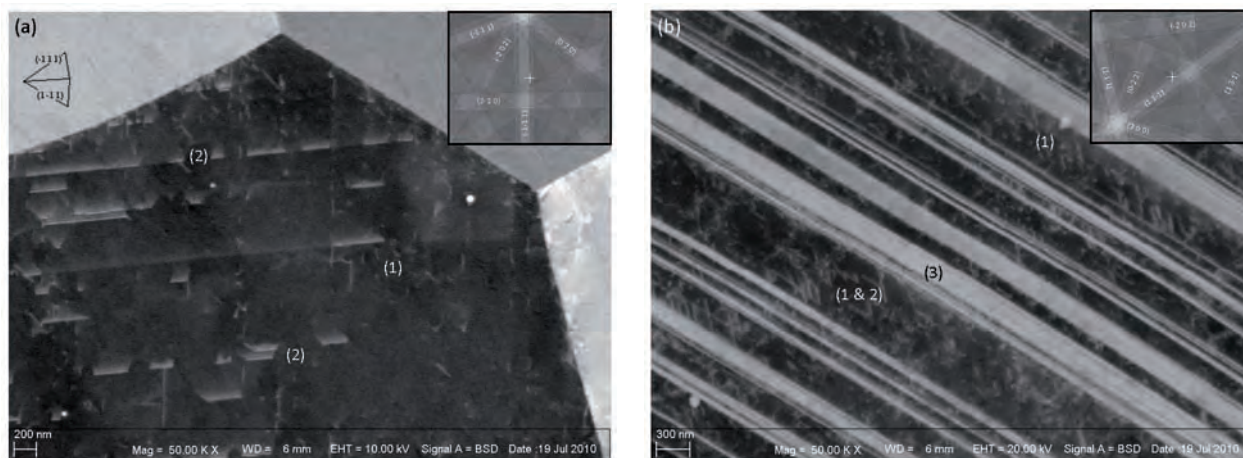itions. The white cross indicates the currently activated diffraction vector. (a) a grain without twinning but well visible stacking faults in a material with very little strain. (b) a grain with intensive twinning in a 7 material with 7 % of plane-strain deformation. (1): individual dislocations; (2): stacking faults; (3) twins.*

the thinnest visible twin in a TWIP steel. At 10 kV it is approximately 15 nm. The maximum depth which is observed in ECCI can be estimated from the visibility of (111) stacking faults in a TWIP steel with fcc crystal structure. From the SF width and its inclination angle a maximum observation depth of about 70 nm is determined for an acceleration voltage of 10 kV on a mainly undistorted lattice. This value is very close to the thickness of usual TEM foils.

The ECCI technique has some significant advantages over the TEM technique which is traditionally used to observe lattice defects. First, it works with semi-bulk samples. This means that there are no thin foil preparation artefacts, like buckling due to stress relieve or loss or creation of dislocations. Also, the preparation may be easier. Furthermore, significantly larger areas can be prepared and observed. The is point is illustrated by Fig. 3, which shows a large overview on the microstructure of a 13 % plane-strain deformed TWIP steel as seen by ECCI. Also, in-situ observations can be performed which are more meaningful than those done on thin TEM foils Finally, the technique requires less complicated equipment. In contrast, the images obtained by the technique do not exhibit a contrast as sharp as those obtained by TEM and the spatial resolution is worse. Nevertheless, we believe that ECCI under controlled diffraction conditions has great potential as a complementary and partly even replacive technique for lattice defect observation.

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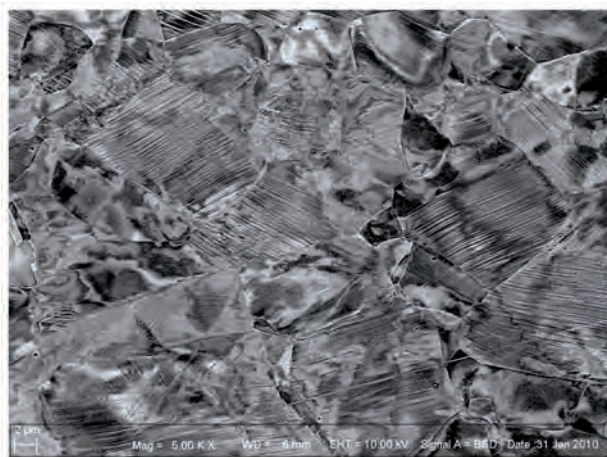**Fig. 3:** *ECC image of a 13 % plane-strain deformed TWIP steel showing an area of approximately 50 x 30 μm² in good orientation contrast.*

Plastic Anisotropy of Single Crystals Revealed by Axisymmetric Indentation

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Single crystal deformation experiments are of fundamental importance in the field of mechanics of microstructures. They can, for example, provide insight into the deformation behavior of the individual constituents and their interactions in multi-phase structural alloys. However, these experiments require a high amount of experimental effort and experience which currently prevents their widespread application and inhibits progress in micromechanical design and alloy development. With the invention of small load indentation devices came the promise to enable the determination of local mechanical properties in microstructures from simple indentation experiments. Progressing towards this goal we present a systematic approach to extract single crystal mechanical properties from axisymmetric indentation testing. In a recent research effort [1,2] this method was developed to investigate the competing deformation mechanisms in the intermetallic phase γ-TiAl. This phase is the major ingredient in light-weight γ-TiAl-based titanium aluminides that will be put into service as blade material in aero-engines in the near future.

Our approach combines experimental and computational techniques into a new tool for rapid quantification of plastic deformation mechanisms at the single crystal level. It is based on the evaluation of the imprint sink-in and pile-up topographies that are formed around axisymmetric indents. For this purpose indents were placed at pre-defined grid points of a chosen region in the microstructure. The orientation dependent surface profiles were measured by atomic force microscopy (AFM). The indented crystal orientations were determined by electron backscatter diffraction (EBSD) [3]. An example of indentation pile-up in γ-TiAl is given in Fig. 1.

The orientation dependent surface upheaval around the indent was simulated by the crystal plasticity finite element method (CPFEM). An elasto-viscoplastic crystal plasticity formulation coupled with a finite element solver was employed [2,4]. By optimizing the constitutive parameters for agreement between experimental and simulated pile-up topographies, the critical resolved shear stresses
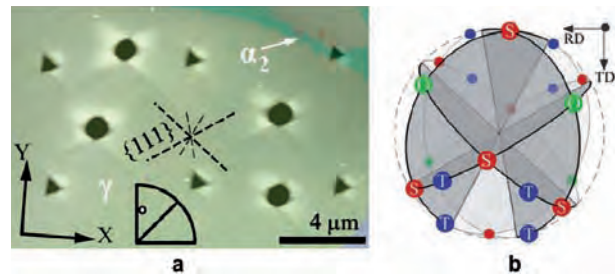
Fig. 1: *Nanoindents in a γ-grain of nearly lamellar Ti-46Al-8Nb (at.-%); a) AFM topographic map (greyscale) combined with an EBSD orientation map ([001] inverse pole figure coloring). The {111}-plane traces coincide with the observed surface steps. Sphero-conical and Berkovich indentations were performed with maximum loads of 6 mN and 3 mN, respectively, and the indentation axis was [1 10 6]; b) Illustration of the crystal orientation of the γ-phase in subfigure (a) (perspective projection): the {111}-planes are shown together with the shear directions for ordinary dislocation glide (O, green), superdislocation glide (S, red) and twinning (T, blue).*

and the hardening properties of the indented material could be extracted.

Because the experimentally measured impression topographies exhibit an arbitrary in-plane rotation for a specific crystallographic indentation direction an in-plane orientation convention was developed. Together with the stereographic projection of the crystallographic indentation axes it results in the novel inverse pole figure of indentation pile-up topographies [2], Fig. 2 (next page). This figure can be used as a reproducible and orientation dependent strain-hardening map of single crystals and it allows one to extract constitutive data that characterize the deformation systems of a given phase.

Dislocation mediated plasticity of γ-TiAl has been investigated in detail by several groups in the transmission electron microscope (TEM) [5]. While providing crucial information about the types and arrangement of dislocations, their main drawback is the lack of good statistics in terms of overall shear contributions if more than one deformation mode can be activated. In contrast, the developed indentation method combines excellent statistical reliability with moderate experimental effort.
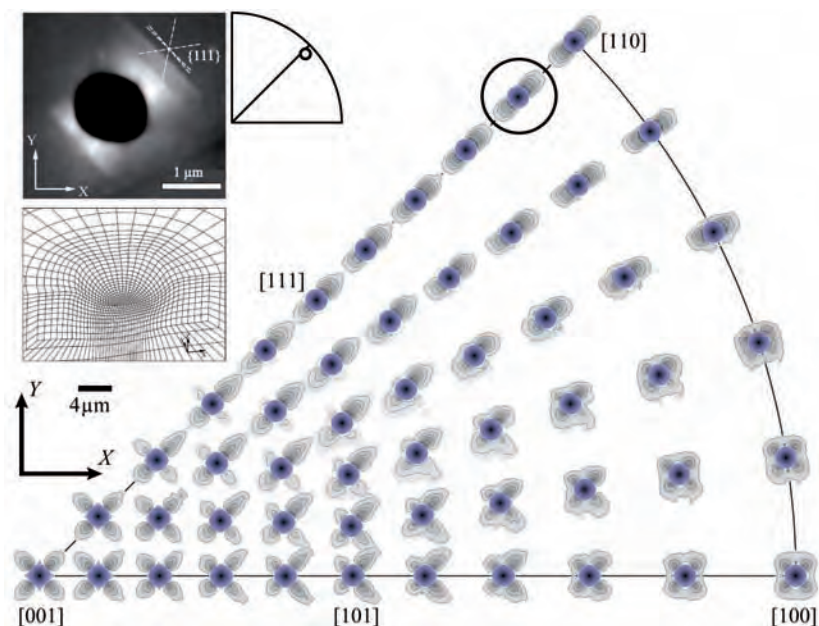
Fig. 2: *Predicted pile-up patterns from axisymmetric indentation in γ-TiAl. The topographic data were obtained from 51 CP-FEM simulations. The individual patterns are placed in an inverse pole figure (stereographic projection) of the respective indentation axes and in-plane oriented according to the developed in-plane orientation convention. Also shown is an experimental pile-up topography for a near [110] indentation (circled) and the discretization of the finite element model.*

Fig. 3 illustrates the distribution of crystallographic shear on a single ordinary dislocation glide system which is highly active for a [101] indentation axis. During our analysis of the orientation dependent piling-up behavior this orientation was identified as characteristic for the relative activities of super-dislocation glide and ordinary dislocation glide. The pile-up analysis identified the easy activation of ordinary dislocation glide as an intrinsic property of γ-TiAl. In conclusion, an efficient method with good statistics was developed to quantify the relative strengths of different deformation modes in crystalline phases via a quantitative and simulation-supported CPFEM analysis method.

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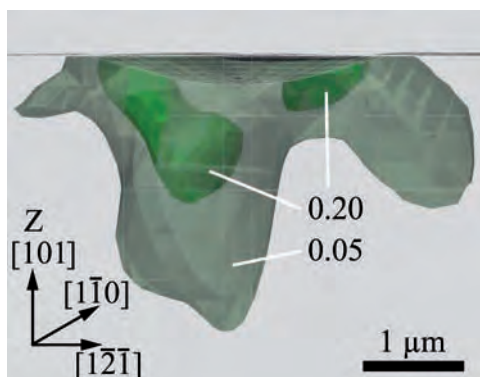
Fig. 3: *Three-dimensional distribution of crystallographic shear on a highly active ordinary dislocation glide system beneath a [101] indentation. Levels 0.05 and 0.20 are depicted by isosurfaces of different saturation.*

Five-Parameter Grain Boundary Character Distribution Analysis via 3D EBSD

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Grain boundaries play an essential role in grain growth, recrystallization, transformation, and deformation. Their structure and properties vary in a 5-dimensional parameter space as a function of misorientation (3 variables) and crystallographic grain boundary plane orientation (2 variables) [1,2]. Hence, it is important to characterize and investigate grain boundary character distributions (GBCD) according to these five variables. The GBCD function specifies the fractions of interface area sections, classified according to the 3 lattice misorientation parameters and the 2 grain boundary normal parameters.

In this study we derive the five-parameter GBCD for an ultra fine-grained Cu-0.17wt%Zr sample, produced by equal channel angular pressing (ECAP) and subsequent annealing at 650°C for 10 minutes from 3D EBSD data sets that were acquired by an automated two-beam system [3]. The instrument is equipped with a field emission electron gun and a Ga^+ ion emitter unit (FIB). The ultra fine-grained CuZr specimen processed by ECAP provides a high density of grain boundaries which is helpful for obtaining good statistics. The 3D EBSD volume probed in this study was about $28×28×17$ μm^3. This data set includes about 91040 boundary segments, which is a robust number for conducting a GBCD analysis [1,2]. The code used for aligning and retrieving the geometry of the grain boundary planes was developed at Carnegie Mellon University by Rohrer and Rollett [1,2,4]. We apply 2 different methods for reconstructing the interfaces in a 3D EBSD microstructure with the aim to obtain the GBCD function directly from discrete 3D topological data sets, namely, the line segment method (LS), and the triangular surface mesh method (TSM). The results are compared to a GBCD function acquired from a statistical 2D stereological approach.

In the first approach (LS) [1] used for calculating the GBCD, the algorithm uses the triple junctions in each 2D EBSD map. The algorithm identifies which triple junctions match among adjacent layers according to the abutting crystal orientations. A triple line then connects the matching triple points in neighboring layers. In the second approach (TSM), the interfacial areas are discretized into triangular area sets, using a marching cube algorithm by which all lines formed by the edges of these triangles will be smoothed. The local grain boundary normal is determined by the cross product of two edge vectors of each triangle. The stereology approach is based on statistics and calculates the GBCD from correlations of 2D EBSD data sets [5].

Fig. 1 shows the misorientation angle distribution and the 3D microstructure as obtained from the 3D EBSD data set. The color code indicates the crystal

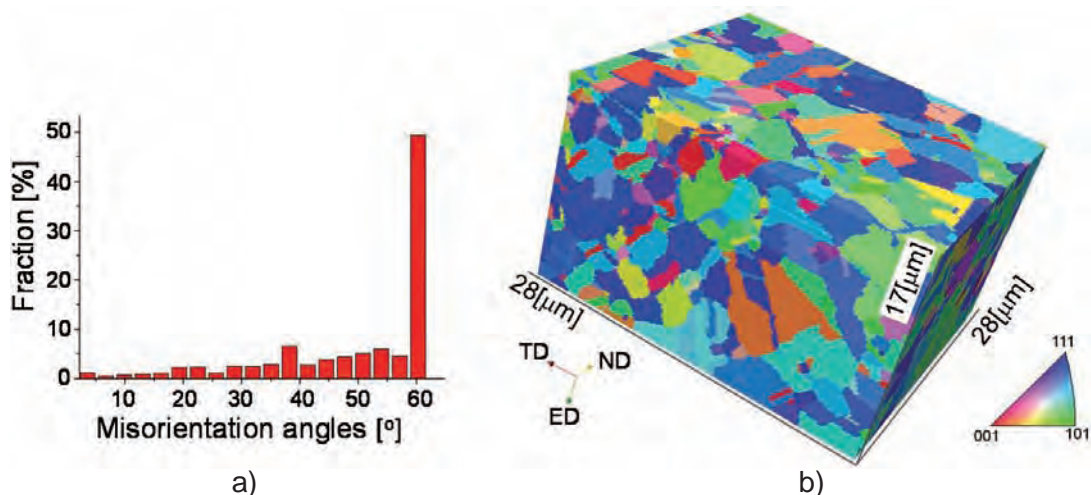**Fig. 1:** *a) Relative fraction distribution for the occurring grain misorientation angles; b) 3D microstructure as obtained from 3D EBSD of the sample after 8 ECAP passes with subsequent annealing at 650°C for 10 minutes. The color code indicates the crystal directions parallel to ED (extrusion direction). Note that the inclinations of the interface planes are not considered in these diagrams.*
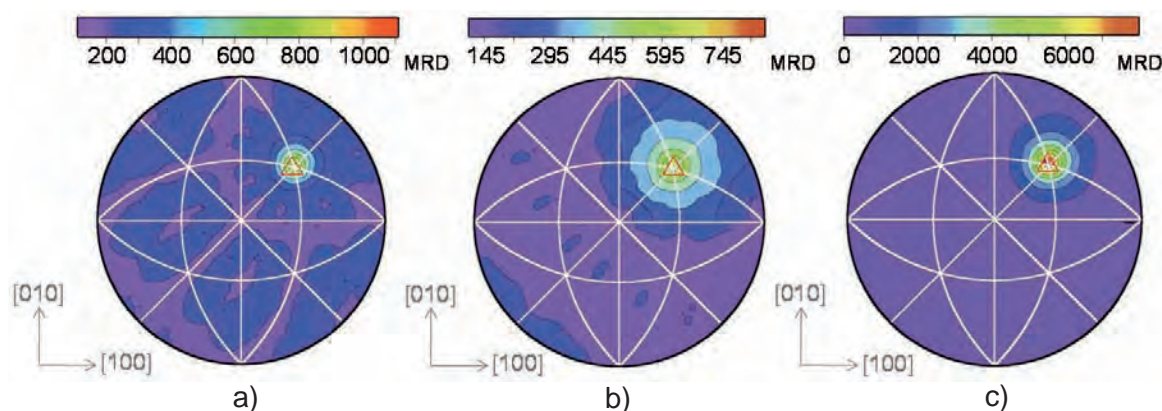
Fig. 2: *Grain boundary plane normal analysis for the 60° <111> twin interfaces according to the a) line segment method (LS); b) triangular surface mesh (TSM); c) statistical stereological approach obtained from 3D EBSD data for the first methods and from 2D EBSD data for the stereology method, for a sample after 8 ECAP passes plus subsequent annealing at 650°C for 10 minutes. Orientation space is discretized into 11 bins per 90° (angular resolution of 8.18°). The red triangle marks the position of coherent twin boundaries. MRD: multiples of random distribution.*

grain directions parallel to ED (extrusion direction). The data set was aligned by minimizing the total disorientation between all voxels in adjacent 2D EBSD layers. For calculating the GBCD function the 5-parameter grain boundary character space has to be discretized. Here, we use for each angular parameter a discretization of 11 bins per 90° (corresponding to a resolution of 8.18°) approximating Brandon's criterion for Σ3 boundaries. We focus on Σ3 twin boundaries, as the misorientation angle distribution of the sample shows a pronounced peak around 60°, Fig. 1a. Σ3 (60°@<111>) boundaries with {111} planes on both sides are coherent twins. As copper has a low stacking fault energy, a high fraction of coherent Σ3 twins can be expected. This is confirmed by the GBCD information shown in Fig. 2 where all three analysis methods reveal a maximum at the {111} interface plane for the Σ3 boundaries.

The maximum peak intensity for the coherent twin is about 1100 and 800 MRD (multiples of random distribution) according to the LS and TSM methods, respectively, Figs. 2a,b, i.e. the two methods provide consistent results. The stereological approach yields about 8000 MRD, Fig. 2c. The deviations between the results obtained by the two direct 3D methods (LS, TSM) and the stereological method is attributed to an overestimation of the background and, hence, to an incorrect normalization in the stereology approach. The other two analysis approaches are not based on statistics (in contrast to the stereological method) but on the direct topological analysis of every single boundary in the microstructure. Consequently, they are more sensitive to the alignment and possible distortion effects between neighboring 2D EBSD maps that are used for the topological reconstruction [1]. Such misalignments may lead to a broadening effect of the boundary plane orientation distribution away from the peaks and to a drop in the maximum (located at the coherent twin boundaries). Fig. 3 shows for some selected grains of the 3D data set shown in Fig. 1b the interface segments in terms of a color coding that indicates their crystallographic normal direction.
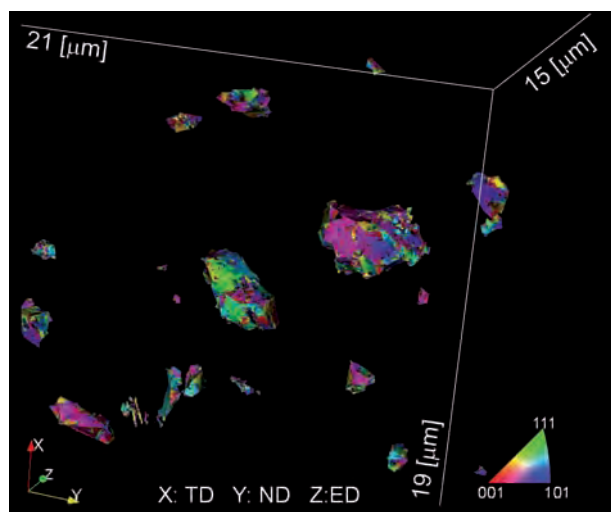
Fig. 3: *20 selected grains of the 3D data set shown in Fig. 1b. The color coding indicates the crystallographic direction of the interface segments (not of the grains).*

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SELECTED HIGHLIGHTS

Identifying and Understanding Hydrogen-related Processes in Steels with Atomistic Resolution

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Hydrogen is known to be responsible for a variety of phenomena in structural materials such as steels. The reason for this sometimes astonishing behavior of the smallest atom in the periodic table is not completely known, even for one of the oldest H-related effects – hydrogen embrittlement (HE). Since its first discovery in 1875 [1] this effect continues to puzzle scientists. The complexity of the problem is primarily related to its inherent multiscale character.

Consequently, almost a dozen of mechanisms were proposed to explain this deleterious effect of H on structural materials. Among them the following are most widely accepted: 1) the formation of voids (bubbles or blisters), 2) the hydrogen-enhanced decohesion, 3) the formation of brittle phases (hydrides or martensites in steels), and 4) hydrogen-enhanced local plasticity. Despite these uncertainties, it is clear that hydrogen practically never acts alone, but interacts with different defects of the crystalline structure, such as vacancies, dislocations and grain boundaries. For example, there is experimental evidence [2] that the trapping of H by vacancies reduces their formation energies, which in turn dramatically affects their concentration. Such superabundant vacancies (SAV) have been observed in a large set of materials, in particularly in steels where they significantly deteriorate mechanical properties, increase the creep rate, cause the formation of voids and reduce crack growth resistance.

In order to understand the effect of defects and microstructure on these phenomena we have de- veloped various multidisciplinary methods describing the hydrogen-metal system on different scales. On the electronic scale, *ab initio* calculations are used to obtain the H potential energy surface (PES) for its incorporation into an austenitic steel. The magnetic structure of these steels is modeled by a double layered antiferromagnet (AFMD). The local minima of the resulting PES represent stable H positions. As an example we mention calculations for bulk Fe-Mn-C alloys, for which not only a preference for the octahedral interstitial sites (OS) over the tetrahedral sites (TS) was found. More importantly, we were able to predict and explain chemical trends for the hydrogen solubility by the volume of the interstitial voids caused by the atomic configuration [3].

Second, we considered the change of the PES due to the presence of vacancies [4] and observed that several of the former octahedral sites now form local minima inside the vacancy (Fig. 1). The solution enthalpy turns out to be lower than for the bulk OS, making vacancies effective trapping centres. Transferring concepts of the well developed methodology of charged defects in semiconductors, a statistical description of the formation energy for H-vacancy complexes as function of the H chemical potential μ_H could be achieved [4]. Fig. 2 reveals the surprising result that for high values of μ_H vacancy complexes with up to 6 hydrogen atoms are energetically most favorable. The situation is similar if Fe is alloyed with other elements such as Ni or Mn. In other materials such as Al and Pb, even up to 15 and 17 H atoms, respectively, can be incorporated.
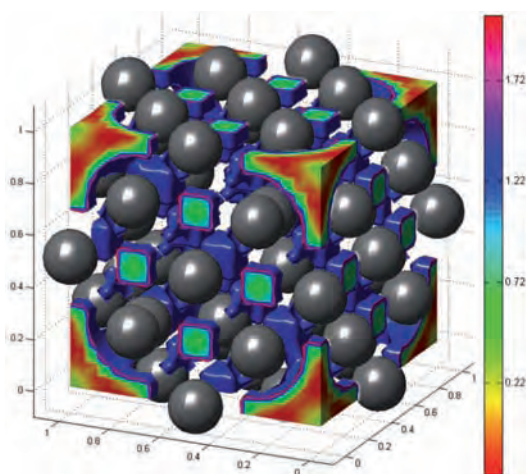

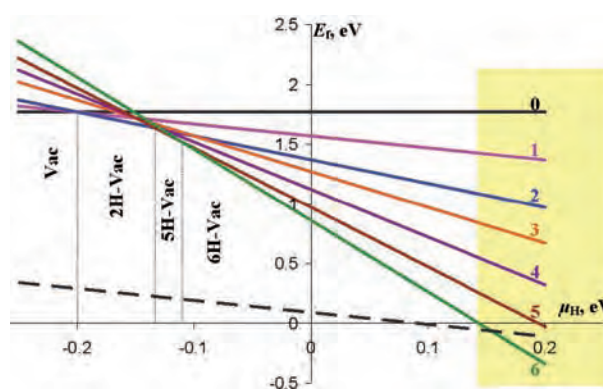**Fig. 1:** *Potential energy surface of H in fcc Fe with vacancies.*

Fig. 2: *Formation energies of point defects in fcc Fe. Dashed line represents interstitial H, solid lines – H-vacancy complexes with number of H atoms shown.*
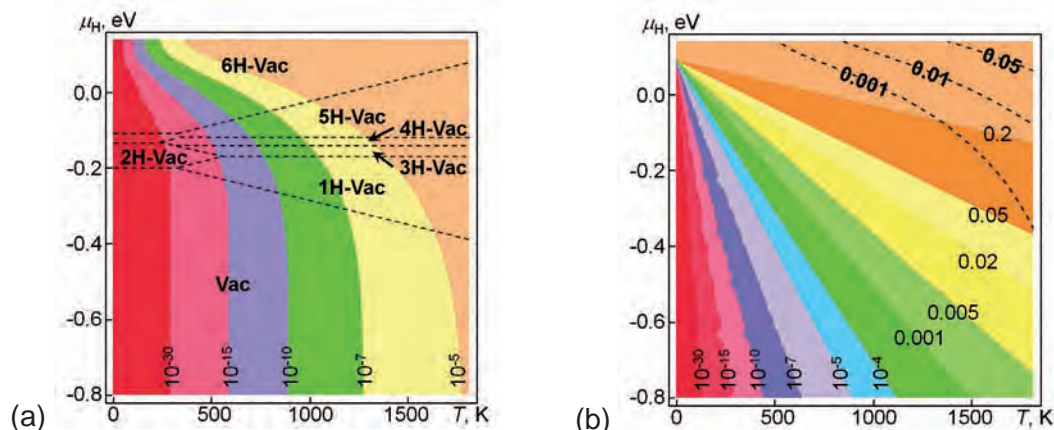
Fig. 3: *a) Vacancy (with the most dominant H-vacancy complexes in dashed regions) and b) H concentration (with ratio of H in vacancies and in interstitial sites shown by dashed lines) in fcc Fe at different temperatures and H chemical potential.*

These features have been accounted for in a thermodynamic model that treats all point defects (empty vacancies, interstitial H, H-vacancy complexes) in metals in a grand canonical ensemble and yields their concentration as a function of temperature and H chemical potential. The resulting concentration of vacancies in AFMD fcc Fe (Fig. 3a) is dramatically affected by the presence of H. Their concentration rises by more than 20 orders of magnitude at room temperature. The inverse effect of vacancies on the H content (Fig. 3b) is, however, rather small and becomes sizeable only at high temperatures and high H chemical potentials.

The solubility of hydrogen in steels can be even more dramatically affected by microstructural defects, such as grain boundaries and dislocations. We have systematically studied both cases for Fe, Ni and other fcc materials. While for the grain boundary the solubility turns out to be highly dependent on its type (misorientation angle, local atomic coordination) [5], the accumulation of hydrogen near an edge dislocation mainly depends on the host matrix material. Using our *ab initio* multiscale simulation techniques we could show that up to 400 times higher hydrogen concentration as compared to the bulk values may occur in its tensily strained region, whenever the hydrogen atoms show an attractive interaction in the corresponding material [6]. The hugely enhanced local concentrations give rise to the formation of dense, hydride like precipitates along the dislocation line which result in a dramatic reduction of the shear stress along the glide plane of the corresponding edge dislocation. As a result dislocation-dislocation interactions are shielded, which is expected to give rise to reduced dislocation separations at dislocation pile-up tips. The increased disregistry, as well as possibly the formation of extended hydride phases at such pile-up structures are likely candidates to induce the formation of cracks and hence the onset of fracture. The above examples may serve as demonstration, how multiscale simulations starting at the *ab initio* level can reveal critical concepts and

details of the atomistic processes underlying HE that were previously not accessible and that nicely complement experimental studies on this topic.

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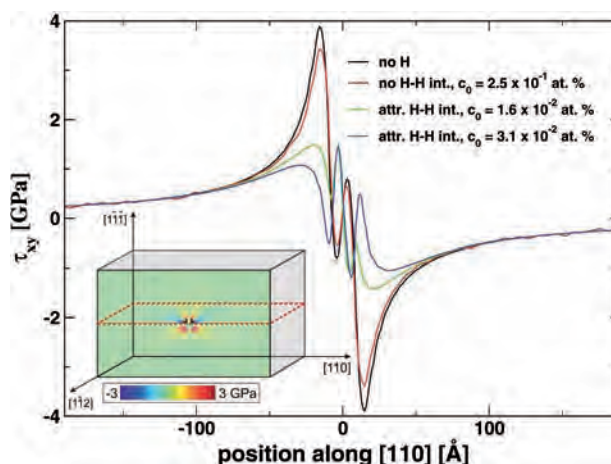
Fig. 4: *Influence of hydrogen on the shear stress along the glide plane (indicated by the red dashed line in the inset) of a {111} $a_0/2$ [110] edge dislocation in Ni. Different H concentrations and the effect of H-H interaction are compared. The change in the shear stress around the dislocation due to the presence of dense, hydride-like precipitates in the tensile strain field of the dislocation is superimposed on the schematic representation of the simulation box.*

Microstructure Characterization and Quantitative Understanding of the Interface Region in Welded Aluminium to Steel Joints

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Metallurgical processes governing microstructure formation in the interface regions of heterogeneous joints are complex and their understanding requires precise characterization under given welding conditions. In this context joints of aluminium to steel are of high interest from an engineering standpoint owing to their huge relevance in current advanced lightweight automotive design solutions and also from a fundamental point of view owing to the intermetallic phases (IMP) that can form in these systems.

One example is the orientation-related growth kinetics of the Al_5Fe_2 phase which is the dominant component in the welded Al-steel interface. Its appearance does not only depend on temperature and time, but it is strongly associated with the presence of other surrounding intermetallic phases.

We can show that only via high resolution EBSD characterization supported by TEM analysis the complete understanding of the interface microstructure is possible.

Fig. 1 shows a larger area of the intermetallic seam of a solid-solid state diffusion couple between low carbon steel and Al99.99 after interdiffusion at 600 °C and 16 h. The phase map shown in Fig. 1a reveals that the main component is the Al_5Fe_2 phase which consists of subdivided grains. The orthorhombic Al_5Fe_2 phase is known [1] to grow faster in a preferential orientation where the *c*-axis of its crystal lattice is parallel to its growth direction. The EBSD inverse pole figure map shown in Fig. 1b provides a clear evidence of the favored growth direction of this phase. Our previous investigations show that
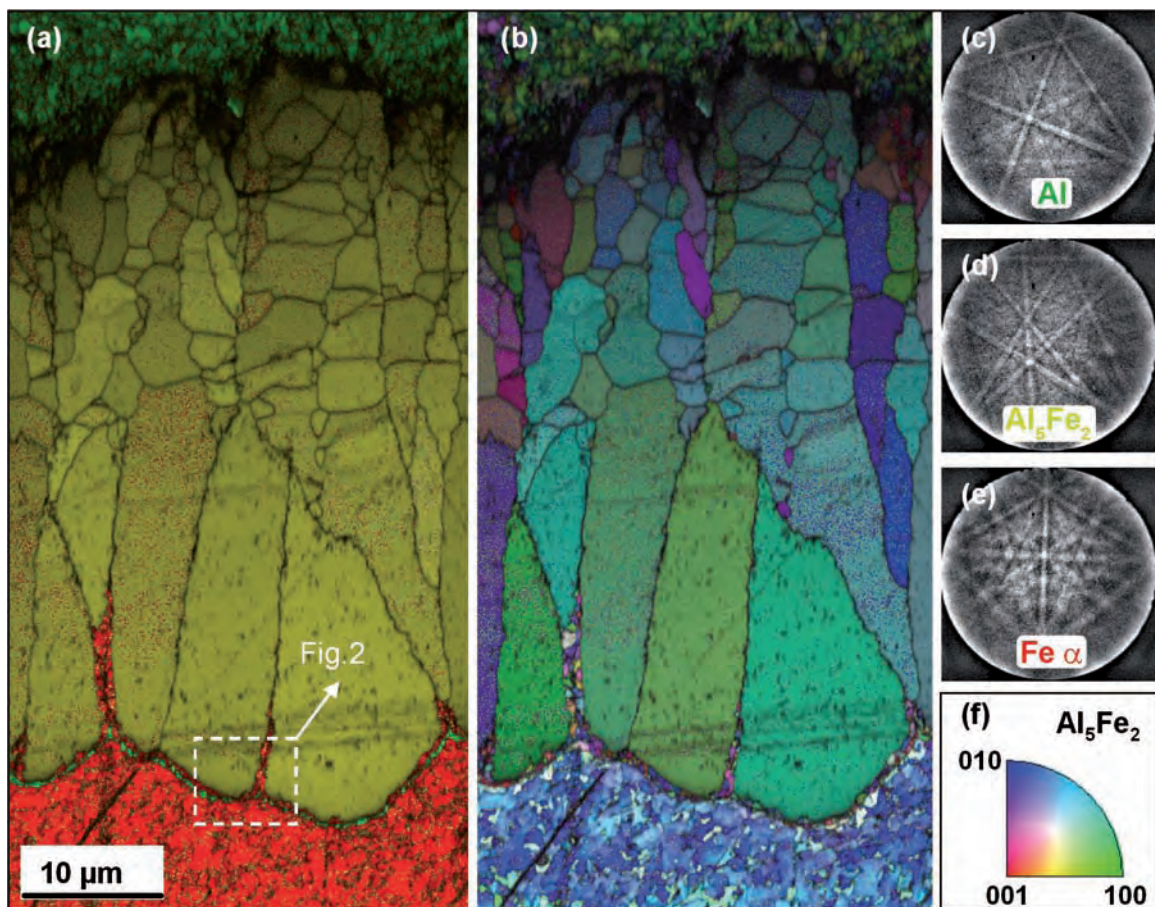
Fig. 1: *EBSD analysis of the IMP-seam developed between low carbon steel and Al99.99 in a diffusion couple at 600 °C, 16 h. (a) Phase map: almost the entire IMP-seam consists of Al_5Fe_2, (b) inverse pole figure map revealing the preferential orientation of the Al_5Fe_2-crystals, (c-e) diffraction patterns, and (f) orientation triangle for Al_5Fe_2.*
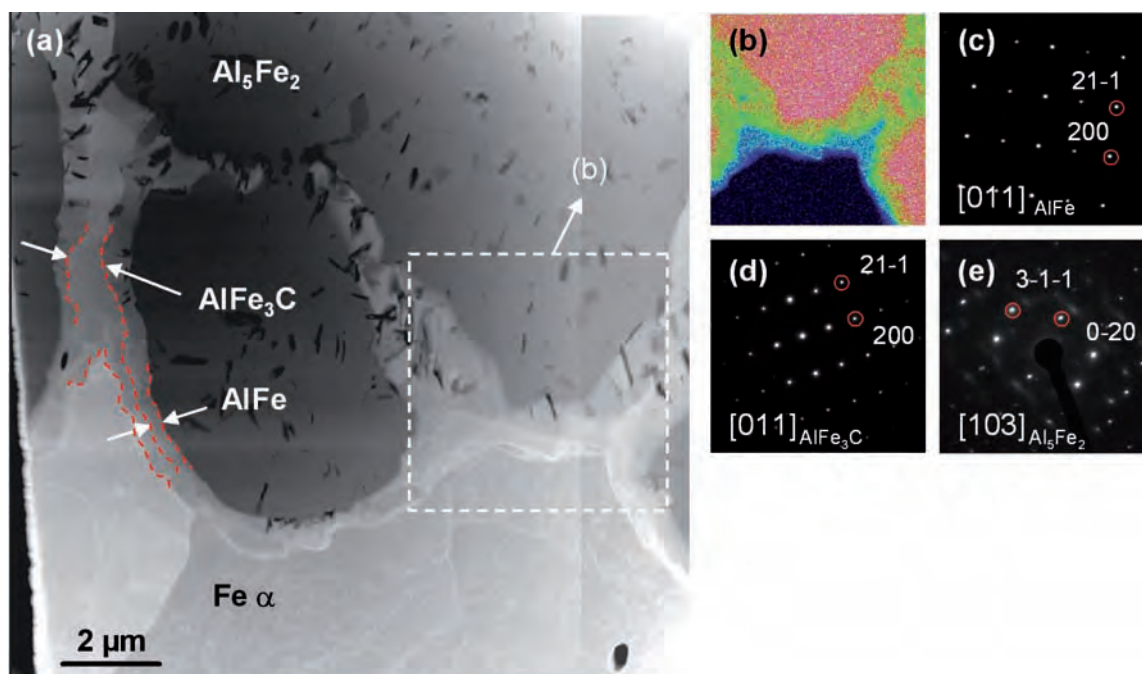
Fig. 2: *TEM analysis of the transition region between Al_5Fe_2 and steel in the diffusion couple from Fig.1. (a) STEM-dark field overview, (b) EDX map of the area marked in (a) showing the Al-content, (c-e) diffraction patterns of the phases.*

Al_5Fe_2 grains of varying orientation nucleate at the growth front as the IMP-layer thickens, but that with increasing annealing time only favorably oriented grains (with the *c*-axis aligned parallel to the material transport direction) grow fast at the expense of less favorably oriented ones. Thus the joint phase and crystallographic information obtained by EBSD provides an important insight into the microstructure formation kinetics of the Al-steel interface.

The thinner area (Fig. 1a) adjacent to the steel is composed of two layers of different phases which are both equally thick independent of the annealing time. Their small size makes phase identification almost impossible and thus TEM must be applied.

Fig. 2 demonstrates the TEM analysis of the transition between Al_5Fe_2 and steel in the diffusion couple from Fig. 1. In the STEM-high angle annular dark-field mode contrast depends mainly on the atomic Z-number of the components. Thus the details of the interface are clearly visible. The EDX map of the area marked in (a) shows that the Al-content of the two phases between Al_5Fe_2 and steel drops successively to 39 at.% and 17 at.% respectively, which would fit to the chemical composition of the phases AlFe and $AlFe_3$, which are to be expected according to the Al/Fe-phase diagram. Selected-area-diffraction (SAD) revealed the following sequence of phases at the IMP-seam: $Al \rightarrow Al_5Fe_2 \rightarrow AlFe \rightarrow AlFe_3C \rightarrow$ steel. The fact that the main component of the interdiffusion layer is Al_5Fe_2 is in agreement with previous work [1] and can be explained by the pronounced growth kinetics of that phase. The presence of the phases AlFe and especially the carbide $AlFe_3C$, however, has not been reported yet. Faster diffusion of C than Fe can explain the formation of $AlFe_3C$ instead of $AlFe_3$, despite the low C content of the steel (0.08 wt.%).

Advanced characterization techniques like EBSD and TEM on specimens which were obtained from specific locations using a FIB procedure, allow a new insight into the evolution and the build up of reaction layers on the Al-steel interface [2,3]. The present results, which show the reaction zones that form during interdiffusion at 600 °C between a low C steel (0.08 wt.% C, European grade: DC04) with Al of 99.99% purity, are a part of the study of the microstructural parameters that govern the reaction kinetics of intermetallic layer growth during interdiffusion between Al and low carbon steel under different conditions.

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Ultra-Sensitive and Spatially Resolved Hydrogen Detection using Scanning Kelvin Probe Techniques

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Hydrogen in steel is a topic of intense research as it plays a decisive role in the applicability and workability of novel innovative high strength steels. One problem is that already very low levels of hydrogen can cause hydrogen embrittlement, which may occur also with considerable delay, making it quite unpredictable and thus very dangerous. Hence, hydrogen uptake and its inhibition as well as ultra-sensitive hydrogen detection are important topics that are addressed within the framework of the CD lab for 'diffusion and segregation mechanisms during production of high strength steel sheet'. Ideally, the hydrogen detection should also provide spatially resolved information on the hydrogen distribution in steels.

This gave rise to the idea for a novel approach for ultra-sensitive and spatially resolved hydrogen detection by use of the Scanning Kelvin Probe (SKP) technique, as hydrogen can cause a change in work function for many metals. For iron or steels it was found that when it was permeated from one side of the sample a work function decrease occurred on the other side, by partial reduction of the oxide layer, i.e. precisely by an induced change in the Fe^{2+}/Fe^{3+} ratio inside the oxide, caused by the hydrogen. However, this turned out to be difficult to reproduce, as the measured values critically depended on the initial state of the oxide and on the atmosphere (even traces of oxygen present in the nitrogen atmosphere caused considerable changes). In a typical permeation set-up usually the exit side is covered by a thin film of palladium in order to enable the exact measurement of the permeating hydrogen by oxidation. We found that a palladium layer evaporated on the surface of

a steel sample is also ideally suitable for detecting the hydrogen distribution by the Kelvin probe method. In Fig. 1 we see the results of a Kelvin probe measurement performed on an iron sample where an area of about 3 mm in diameter was cathodically charged with hydrogen, and a palladium film of about 200 nm thickness was evaporated onto the surface. Due to the difference in the chemical potentials between palladium and iron, the palladium film takes up hydrogen from the underlying iron. There where more is stored inside traps, i.e. where the iron was cathodically charged with hydrogen, a steady flow of hydrogen into the thin palladium film leads to a steady enrichment of hydrogen in the palladium above these active sites in the iron. As will be shown, the dependence of the work function of the palladium on hydrogen concentration shows a linear dependence, just like it is already well known for hydrogen charged palladium in electrochemistry within the α-phase region [1]. In these experiments it was found that the electrode potential of the palladium follows the Nernst equation, i.e. more precisely $E = + RT/2F \cdot \ln([H^+]^2/p_{H2})$, which, at a given constant pH and considering the equilibrium $H_2 \leftrightarrow 2 H_{ad} \leftrightarrow 2 H_{ab}$, can be expressed as $E = E_0 - RT/F \cdot \ln([H_{ab}])$. This can be shown in highly viscous electrolytes [1], where the loss of hydrogen is suppressed.

We found here that the hydrogen in the palladium in nitrogen atmosphere shows more or less no tendency to escape when the SKP measurement is performed in dry nitrogen atmosphere. This becomes quite clear from Fig. 2. Here the results obtained from the following experiment are shown: on one side
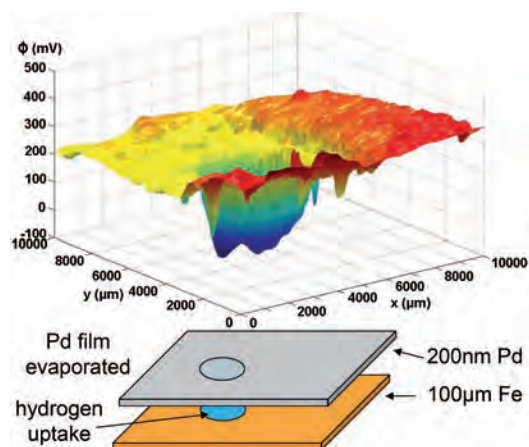

Fig. 1: *SKP map obtained on a Pd film covered iron foil where a spot of about 3mm in diameter was cathodically charged with hydrogen.*
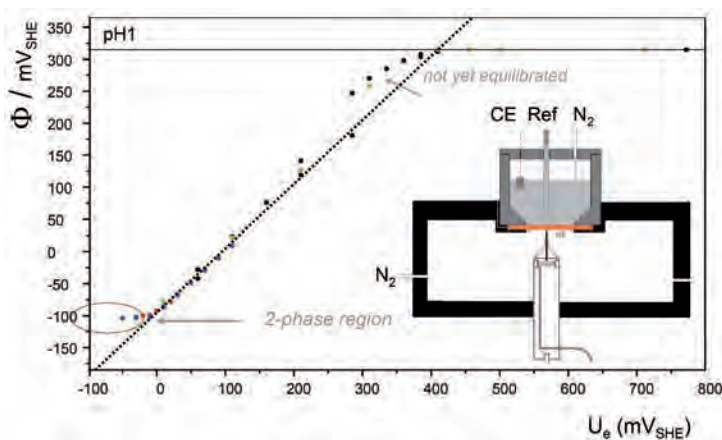

Fig. 2: *Work function on the exit side of a 25 micron Pd membrane, polarised at the entry side to different potentials (sulphuric acid, pH 1); different colours stand for different series of measurements.*
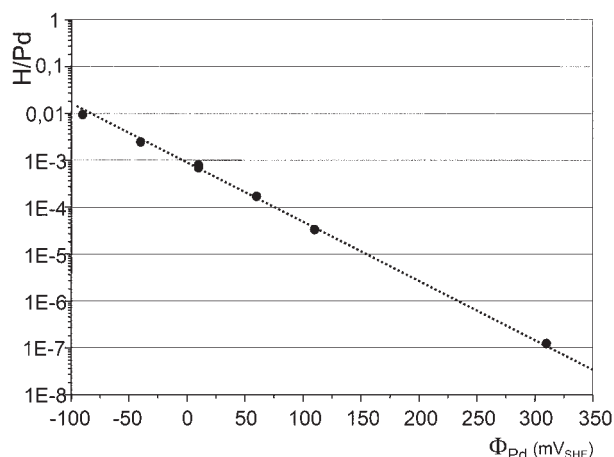
Fig. 3: *Correlation between concentration of dissolved hydrogen within the Pd and the work function resulting from this.*

Fig. 4: *EBSD map of a polycrystalline Pd membrane and optical image (mirrored!) of the AFM tip on the sample, with indication of some grains.*

a palladium membrane was polarized to different potentials, on the other side the resulting change in work function was measured, in Fig. 2 given as potential vs. SHE [2]. As can be seen a linear behaviour with slope one is observed in a wide range (after sufficiently long waiting times). This indicates that the hydrogen concentration has reached the same level over the whole sample and especially, that exit and intro side seem to be in equilibrium, indicating that only very negligible hydrogen desorption occurs on the exit side. The amount of dissolved, i.e. available, hydrogen in the palladium in equilibrium with a certain applied potential can be measured by anodic potential step experiments, evaluating the charge under the resulting current transient showing the hydrogen that is anodically consumed by oxidation to H⁺. In Fig. 3 the dependence between concentration of dissolved hydrogen in the palladium and the resulting work function, given as electrode potential vs SHE, is shown. The observed dependence does not follow exactly the Nernst equation, as the slope is more than 60 mV per decade, similar to the results obtained by Yang and Pyun [3]. This is most likely due to strain and the presence of trap sites within the palladium membrane [4]. This result shows that the amount of hydrogen

Fig. 5: *Surface potential maps obtained on the two grains. Note that a higher surface potential means a lower work function/electrode potential.*

inside the palladium can be measured down to concentrations of less than 0.1 at-ppm, i.e. we have a really extremely sensitive and also spatially resolved (Fig. 1) detection method!

These results also mean that the work function on Pd, which should depend also on the crystal orientation, will be independent of this as soon as the hydrogen content starts to determine its value, i.e. in the 0.1 ppm range. This was shown within another project (C. Senöz, SURMAT and DFG) by applying SKPFM (Scanning Kelvin Probe Force Microscopy, an AFM based technique for measuring the surface potential). First an EBSD map was obtained from a polycrystalline Pd sample (Fig. 4). Then this sample was charged with hydrogen from one side and the surface potential of two grains (one (111) and the other close to (101)) was measured. As can be seen the contrast in potential between the grains was lifted due to the hydrogen uptake (measurement in nitrogen atmosphere), and restored upon hydrogen depletion in air (Fig. 5).

To make use of this sensitivity of the work function of palladium for studying hydrogen in steels is subject of current research, making use of evaporated thin films of Pd and the lower chemical potential of hydrogen in Pd.

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S E L E C T E D   H I G H L I G H T S

Scanning Kelvin Probe Microscopy for *in-situ* Detection of Synchrotron-Radiation-Induced Changes at Surfaces and Interfaces

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A wealth of information on surfaces, interfaces and thin films can be derived from reflectivity and scattering studies using highly brilliant synchrotron radiation (SR). However, in such studies the inter-action of the intense X-ray beam and the sample can lead to side effects, such as the accumulation of charges at the surface, changes in the surface structure and chemistry or even generation defect structures. For example, the breaking of the sym-metry at interfaces of biological molecules can lead to complex equilibrium electrostatics with high local fields. Electric fields at an interface are important for many physical, chemical and possibly biological properties. But these electrostatic fields are difficult to measure. The great advantage of the Scanning Kelvin Probe (SKP) is that it enables the in-situ measurement of the work function (or dipole potential) at surfaces and buried interfaces of many layered systems [1-3]. Hence, a fundamental study on typical materials for synchrotron radiation based reflectivity and scattering studies were performed at the high energy undulator beamline ID15 (ESRF) measuring the structural and electrochemical properties simultaneously by means of X-ray scattering and a special constructed SKP, respectively.

In Fig. 1 a typical X-ray reflectivity under ambient conditions of a sapphire (0001) single crystal is shown. Simultaneously with the increasing photon flux at the illuminated sample surface a huge change by more than 2 V in the Volta potential difference at the illuminated sample area can be observed, giving evidence of radiation induced accumulation of charges at the surface. After stopping the irradiation these accumulation decays within 900 s reaching the former potential level.

Such kind of accumulation of charges can be directly influenced by the chemistry, functional groups and termination of the surface. To study these effects in more detail p-type silicon (100) wafers were cleaned by acidic and alkaline piranha solution to generate surfaces with positive and negative charged functionality, respectively (see Fig. 2e-f). Depending on the termination of the surface one has fixed negative or positive charges on the surface and matching charges originating from the ambient as mobile ones. The air ionized by the 3rd generation undulator radiation generates additional mobile charge carries that result in an effective negative charging in the case of the acid piranha cleaned wafer (agglomeration of negative charges) and an effective positive charging in the case of the alkaline cleaned one. As soon as the SR-beam hits the surface photoelectrons are ejected from the surface leading to a positive charging (e.g. cathodic shift of the potential). Additionally, the X-ray beam changes the surface chemistry by wiping out most or all functional
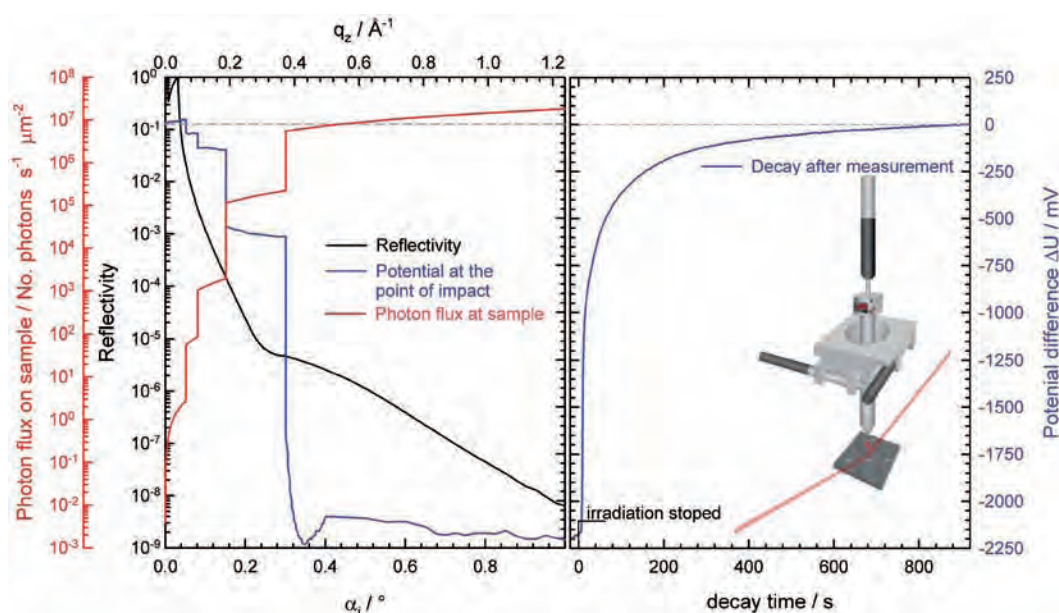
Fig. 1: *Combined in-situ X-reflectivity and SKP measurement. The reflectivity (black curve) was measured at E = 69.81 keV. The SKP measurement (blue curve) was performed at the point of impact of the incoming X-ray beam, like shown in the insert. The photon flux of the illumination X-ray beam is shown in blue.*
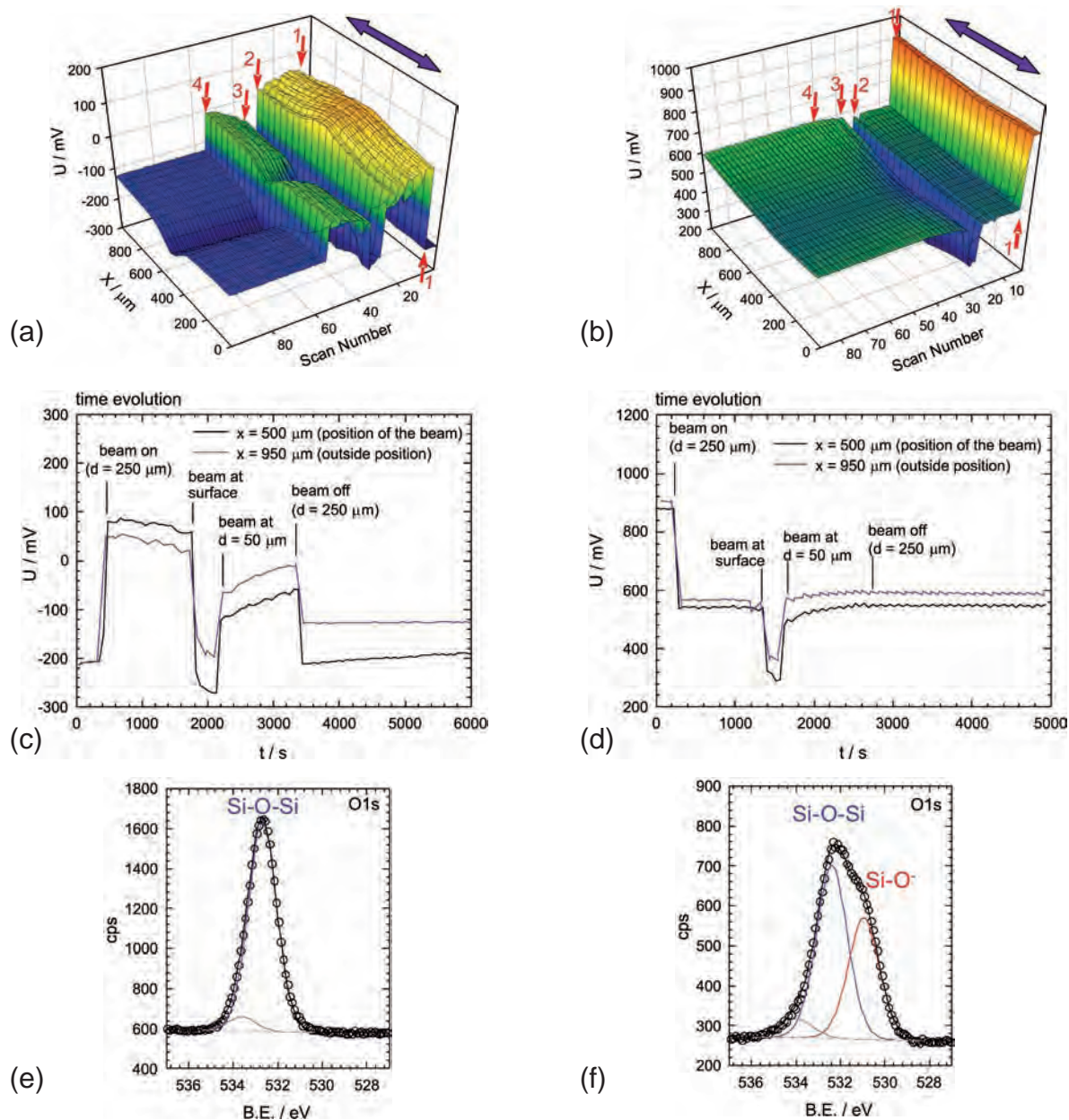
Fig. 2: *Continuous SKP line scans during irradiation of the acidic (a) and alkaline (b) piranha cleaned p-type Si wafer. The trajectory of the 25 µm x 5 µm beam moves parallel to the sample surface along the x = 500 µm coordinate while the scan direction of the SKP is dissipated by the blue arrows. The illumination started at a depth of 250 µm below the surface (1), the beam is moved to the surface till it hits the surface (2), moved back (3) into a depth of 250 µm, and the illumination is stopped (4). The time evolution of the Volta potential difference of the illuminated and untouched area of the acidic and alkaline piranha cleaned Si wafer is shown in (c) and (d), respectively. High resolution O1s XPS spectra measured at a take off angle of 10° of the acidic and alkaline piranha cleaned Si wafer are shown in (e) and (f), respectively.*

groups at the surface. As consequence the density of fixed charge groups in the area illuminated by the X-ray beam is changed, leading to different potentials between the illuminated and untouched area of the sample, which can be of permanent nature.

In summary, we have shown that the SKP is not only applicable to monitor in-situ undulator beam induced changes at the surface, but also the presented results show that indeed the undulator beam affects the structure and electrostatics at the surface by the accumulation of charges, elimination of surface functional groups and generation of photoelectrons.

Such results on (reversible) beam-induced changes via changed electrostatics are of prime importance when e.g. studying soft (bio)molecular interfaces with hard X-ray radiation.

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Real Time Monitoring of Dissolution Processes Using a Microelectrochemical Scanning Flow Cell

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The steady progress in material science and the development of new coating materials has an immediate consequence for corrosion science: The complexity rises drastically. With increasing number of components in modern alloy systems, the field of electrochemistry thus faces extensive challenges. Identifying the influence of each particular component in order to derive promising pathways for material optimization [1] becomes more than substantial. Moreover, most surfaces are not uniform in elemental distribution and phase composition, and these microstructural aspects are playing a major role besides the bulk composition itself [2].

To address these challenges, three key approaches have been combined in one single electrochemical experimental setup of a flow type scanning droplet cell (SDC). A high spatial resolution is achieved by a capillary cell which confines the investigated area down to a diameter of around 200 µm. This typical SDC feature was extended by a continuous electrolyte flow that additionally provides a controlled mass transport of reactants and products and the possibility to couple various analytical methods in the off stream, e.g. in the present case a high sensitivity UV-VIS setup (Fig. 1). Last but not least, by consequently aiming for complete computer control, high throughput experiments have become possible that require no user interaction during automated screening of surfaces.

The potential of the complementary combination of high throughput electrochemistry and real time analysis is demonstrated by the investigation of
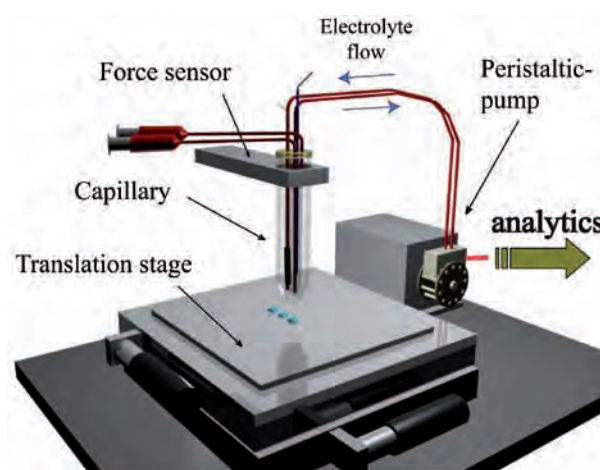
Fig. 1: *Schematic drawing of the f-SDC setup with a two compartment capillary (theta type).*

zinc coatings, where the parameter space created by environmental conditions is extensive and the dissolution mechanism of zinc highly complex by itself [3]. Fig. 2 shows the online Zn detection during a 1000 s open-circuit potential (OCP) measurement in borate buffers of two different pH values with a subsequent anodic sweep (2 mVs^{-1}).

It is obvious that the dissolution profile reaches a plateau value during the OCP scan which reflects a steady removal of zinc by the streaming electrolyte. The magnitude of zinc dissolution is proportional to the proton concentration in solutions of near neutral pH and is not reflected by the corrosion potential
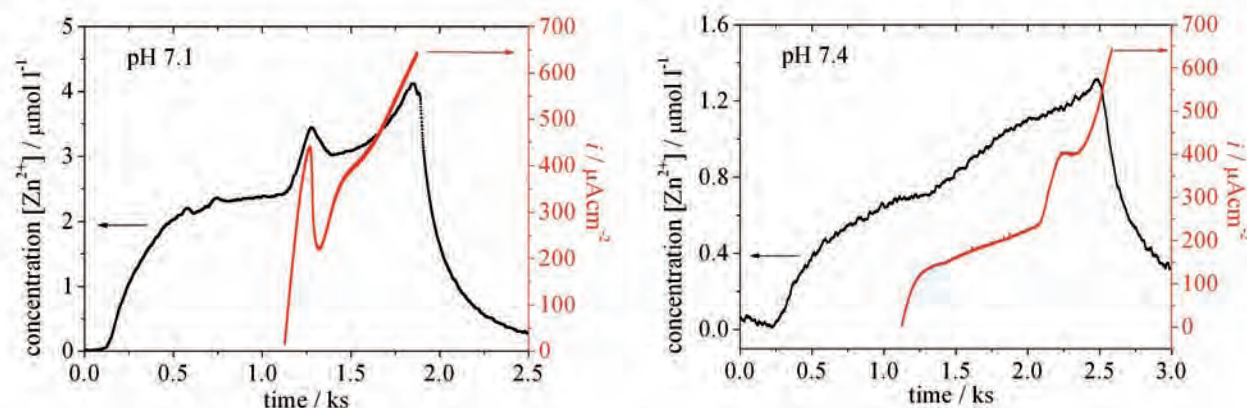
Fig. 2: *Combined OCP-anodic sweep experiments with online zinc detection.*
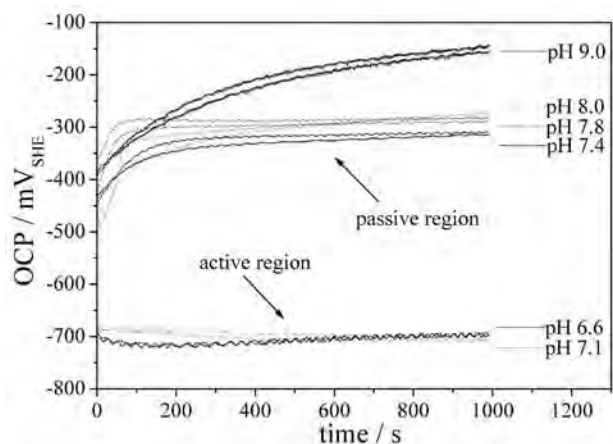
Fig. 3: *OCP measurements of pure Zn in borate buffers of various pH.*

at all, which rather depends on the integrity of the passive film formed on the surface. The OCP transients recorded over 1000 s as shown in Fig. 3 demonstrate a clear distinction between the active and passive region or, in other terms, an incomplete (active) or complete (passive) coverage by the passive layer [4]. The real time dissolution monitoring provides reliable information with high relevancy for predicting corrosion resistance of coatings that is not accessible by traditional approaches.

In an effort to verify the feasibility of high throughput screening experiments, laterally graded Zn-Mg material libraries were prepared by thermal PVD [5] and investigated by means of dissolution monitoring, i.e. OCP measurements and anodic sweeps as previously shown in Fig. 2. A high consistency along the composition gradient has been observed with clear indication of a non-linear dependency between electrochemical activity and magnesium content. Fig. 4 shows a 3D plot of (a) the anodic sweep and (b) the OCP along the composition gradient. In agreement with previous investigations [3], extraordinary behaviour has been observed around a composition of 80 at. % Zn, which manifests in low OCP values and low Zn dissolution, but high passivity current during anodic scans. Furthermore, oxygen evolution became dominant over film breakdown between 6 and 9 at. % Mg at high potentials. This is assumed to originate from the formation of $MgZn_2$ intermetallics at the surface identified by grazing incidence X-ray diffraction performed along the sample gradient.

In summary, a fully automated setup for electrochemical experiments with integrated real time product analysis has been developed, enabling combinatorial investigations of material corrosion.

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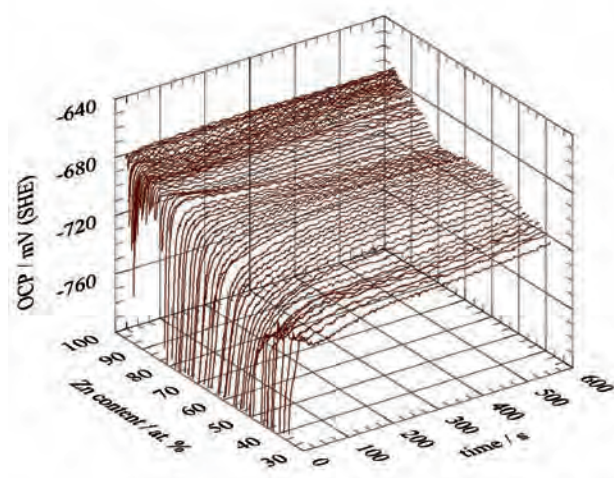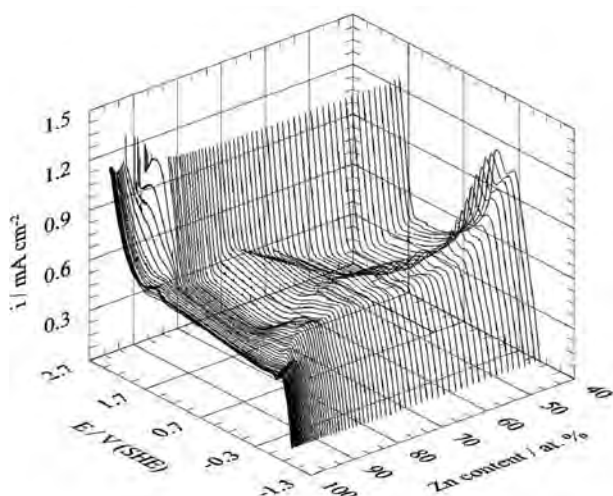
Fig. 4: *(a) Anodic sweeps starting at OCP along a Zn-Mg gradient and (b) OCP measurements in borate buffer pH 7.4 under constant electrolyte flow (15.6 µl min^{-1}).*

Design of Systems for Spectroscopic Studies of the Metal/Electrolyte Interface

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The main challenge for analyzing metal/electrolyte interfaces with in situ optical spectroscopy is the delivery of light to the examined interface [1]. Because both the electrolyte and metal attenuate the intensity of light through absorption, methods for increasing the intensity at the surface under study need to be developed. In the infrared spectral range, the absorption is particularly strong. Here, we are discussing two approaches to solve this issue for infrared light. Both use a high-refractive index semiconductor as medium of incidence, on which metal is deposited and brought into contact with a solution. The first approach increases transmission through continuous metal films. The second approach uses small metal particles at the surface and therefore offers a path towards designing a well-defined, rough model interface.

The first approach is depicted in Fig. 1. It follows a concept introduced earlier for visible light [2]. A continuous and smooth metal film usually obstructs the propagation of infrared light into the electrolyte (Fig. 1, left) [2]. Two new effects are observed when introducing a high-refractive index, transparent, anti-reflecting interlayer into the system (Fig. 1, right) [3].
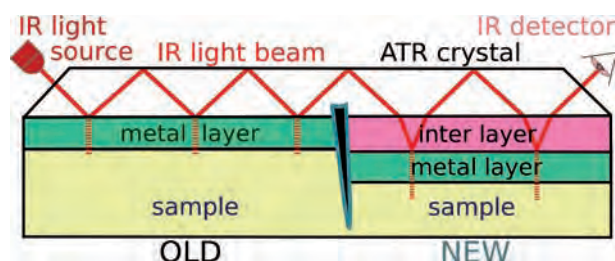
Fig. 1: *Comparison of the traditional use of thin metal films in internal reflection spectroscopy (left) and the new concept using an antireflective interlayer between metal and medium of incidence (right).*

The interlayer increases the light intensity at the metal/electrolyte interface [2]. Therefore, enhanced absorption of the liquid sample in contact with the surface is observed. The enhanced absorption occurs at certain wavelengths which depend on the medium of incidence, the thickness and refractive index of the interlayer, and to a lesser extent on the angle of incidence. Enhanced absorption is observed in minima in the reflectivity spectra. As an example, Fig. 2 shows the dependence of the reflectivity on wavenumber and angle of incidence for the system ZnSe - Ge (1350 nm) - Au (20 nm).
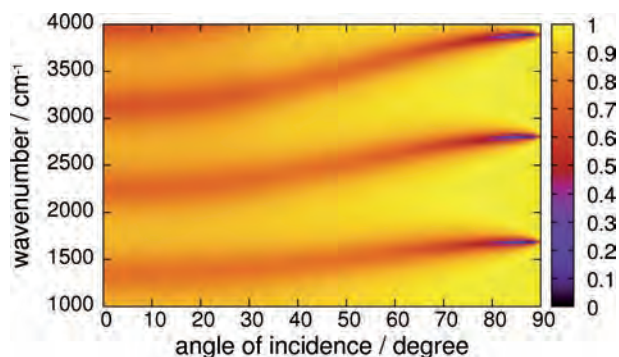
Fig. 2: *Reflectivity of the system ZnSe-Ge(1350 nm)-Au(20nm)-Air as function of wavenumber and angle of incidence. The reflectivity scale is given on the right.*

The plot shows bands with minima in reflectivity. While the wavenumbers of the minimum only weakly depend on the angle of incidence, the reflectivities at the minima are lower at high angles of incidence. For studying the effects of the interlayer on the absorbance of a sample in the presence of a 40 nm gold layer, an angle of incidence of 45° was chosen. The "test sample" was the organic solvent acetonitrile. Spectra with s-polarisation of the region of the CN stretching mode in the presence and the absence of the interlayer are presented in Fig. 3. While in the absence of the interlayer, only a baseline is observed, the sample absorption is clearly present when the interlayer was deposited [3].

The infrared-transparent interlayer furthermore acts as an interference coating. The interference pattern is clearly visible in the reflectivity data presented in Fig. 2. In absorbance spectra, an interference
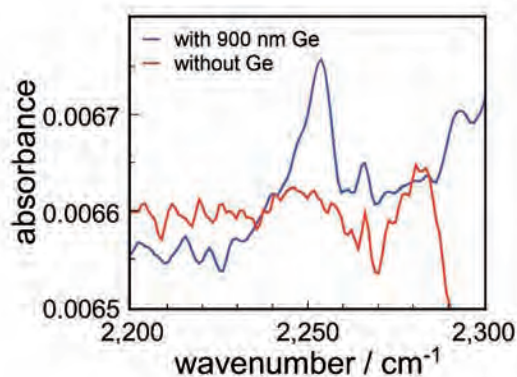
Fig. 3: *IR spectra (CN stretching mode region) of aceto-nitrile on gold in the presence and absence of the germanium interlayer.*
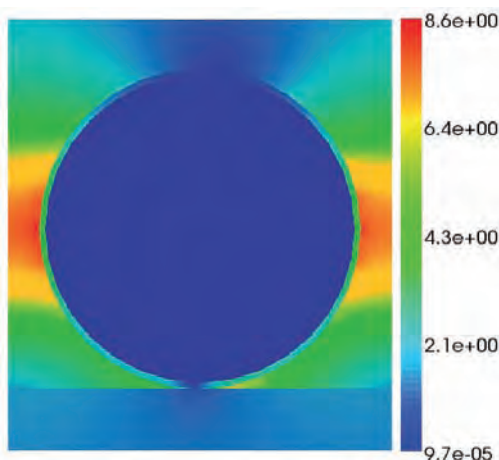
Fig. 4: *Electric field strength in V/m around a gold cylinder. An incoming plane wave at 45° incidence angle in silicon (bottom) generates an evanescent wave which is used to generate the fields around the metal nanostructure.*

pattern is also visible if the real part of the refractive index of the sample in contact with the metal layer is different from the real part of the refractive index in the background measurement. These interference fringes therefore contain further analytic information about the refractive index of a sample. On a hemispherical CaF_2 substrate, the dependence of the interference pattern on the angle of incidence with an acetonitrile sample was studied both experimentally and by computation. The wavenumber positions of the maxima and minima agree quite well between computation and measurement. Certain angles of incidence are observed where the sign of the bands changes. These angles can be predicted numerically with good agreement to the experiment. The exact height of the peaks does not agree with computations. The peak "absorbance" is higher at higher angles of incidence, with less agreement between theory and experiment.

In situ studies of rough surfaces are still difficult with many optical techniques, especially if quantitative or at least semiquantitative information is required. The difficulties arise from the fact that it is hard to relate to observed absorbances or emission intensity to a number of molecules, as the field strength of the electromagnetic fields at the different parts of the complex interface are hard to access. On the other hand, infrared absorption and Raman spectra both show signal enhancement in the presence of certain surfaces. The problem in these surfaces is that near "hot spots", molecules near the surface contribute strongly to the overall spectrum, while no contribution to the spectrum can be observed from other regions of the surface. A quantitative understanding of spectra from such surfaces is only possible if detailed computations of the spectra of metal particles near a surface can be performed. We

are using the finite element method (FEM) to solve the time-harmonic Maxwell equations in order to obtain electric fields near surfaces and subsequently compute surface enhanced infrared absorption spectra. An image of the electric fields around a gold particle in a periodic array stemming from the periodic boundary conditions is displayed in Fig. 4, while computed spectra of an organic layer under particles with different diameters is shown in Fig. 5. The field image around the particle for p-polarised incident light shows that the field strength is large in the region between particle and surface, as well as between the particles. In the region between particle and surface, enhancement factors between 50 and 100 are obtained. Furthermore, the enhancement increases with increasing size of the particle in both s- and p-polarisation, and is particularly strong in p-polarisation. If one is able to manufacture surfaces with well-defined morphologies, quantitative spectroscopic studies could be possible coupled with simulations.

Overall, the concept of the interlayer introduced above assists the study of planar interfaces, while quantitative spectrum simulations for rough surfaces show interesting perspectives to study, with high sensitivity, regions which are hard to access otherwise. Having developed both approaches, the application to study molecules near interfaces as well as the stability of interfaces are next steps.
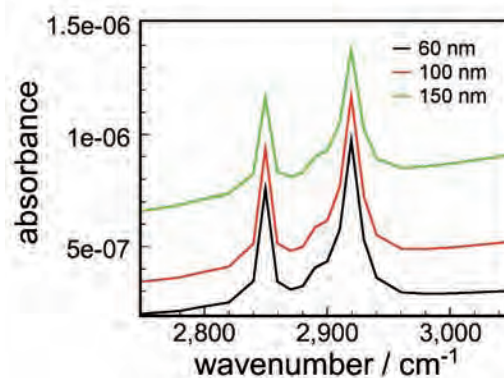
Fig. 5: *Computed surface-enhanced infrared absorption spectra from an organic layer with poly(ethylene) optical constants under gold particles of three different diameters.*

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Towards Electrochemistry from First Principles:
Thermodynamics of Ions at the Interface

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The corrosion of steel is a complex phenomenon that involves processes at many different length and time scales. At present our understanding of the key steps, let alone their interplay, is incomplete since they depend on the material composition, the environment, the pre-treatment, and many other aspects that may influence the speed and course at which corrosion evolves. At the fundamental scale, the metal reacts with oxidising species to form a surface oxide in a multi-step electrochemical reaction. The nature of the reactive intermediates and their exact place within the reaction chain continues to be a subject of heavy debate. These questions can be systematically addressed by determining the thermodynamics and kinetics of the surface, as well as of the ions in solution and in the oxide layer.

In this context, *ab initio* electronic structure calculations offer a complementary view to experimental investigations. A key to the success are surface phase diagrams, which identify the thermodynamically preferred surface termination as a function of chemical potentials. The availability of such diagrams allows to reduce the multitude of fast processes and the identification of the thermodynamically stable surface phases thus providing the basis for determining the critical reactions taking place at the interface.

Surface phase diagrams rely on an accurate determination of free energies at finite temperatures. Using the techniques developed in the Department of Computational Materials Design for bulk phase diagrams, we were able to extend the methodology to surfaces. In a collaboration with the Department of Interface Chemistry and Surface Engineering we employed this extension to study the passivation layer of Zn-coated steels. Specifically, we investigated the morphology of the polar ZnO(0001) surface in dry and humid oxygen environment. Vibrational contributions to the free energy become decisive in the competition between various surface phases to gain thermodynamic stability [1]. However, when it comes to explaining all experimental observations of surface geometries and phase transitions in different environments, conventional phase diagrams fail to predict the appearance of meta-stable phases. We therefore generalized the concept of equilibrium surface phase diagrams to include kinetically stabilised structures [2].

Fig. 1 shows two examples of such extended surface phase diagrams. The key idea is to extend the phase diagram beyond the thermodynamically allowed region of H-chemical potentials. As a consequence the upper limit is no longer pinned to the formation of H_2 molecules and a number
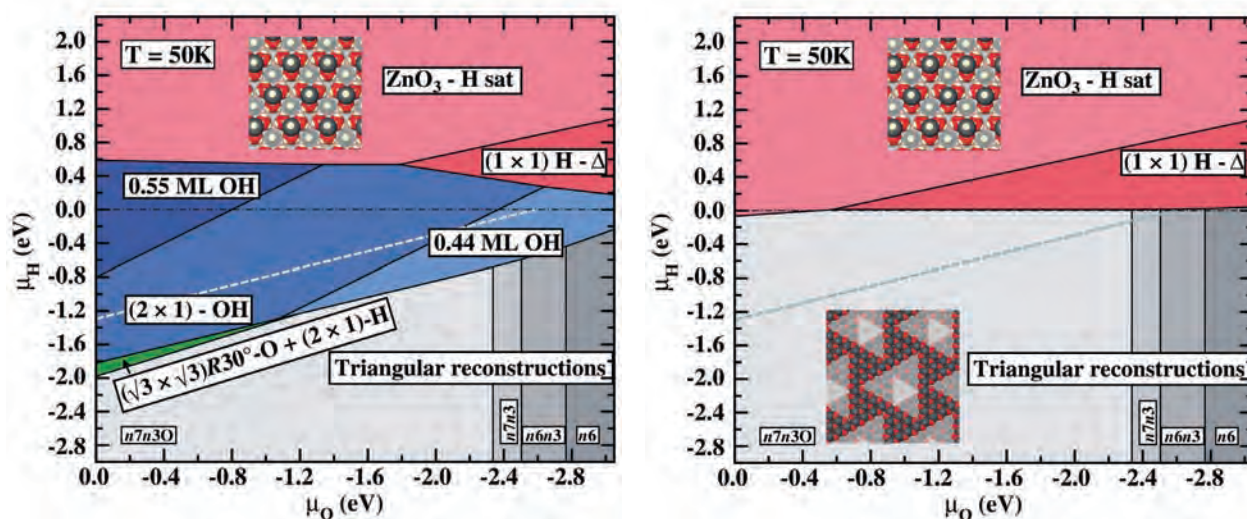
Fig. 1: *Extended phase diagrams for ZnO(0001)-Zn. Regions outside the thermodynamically allowed region for H chemical potentials are found above the dot-dashed black line, in which also H-adsorbate structures are found. Hydroxylated surface structures have been removed from the meta-stable phase diagram (left), since their formation might be kinetically hindered on a surface characterized by pre-existing triangular reconstructions.*
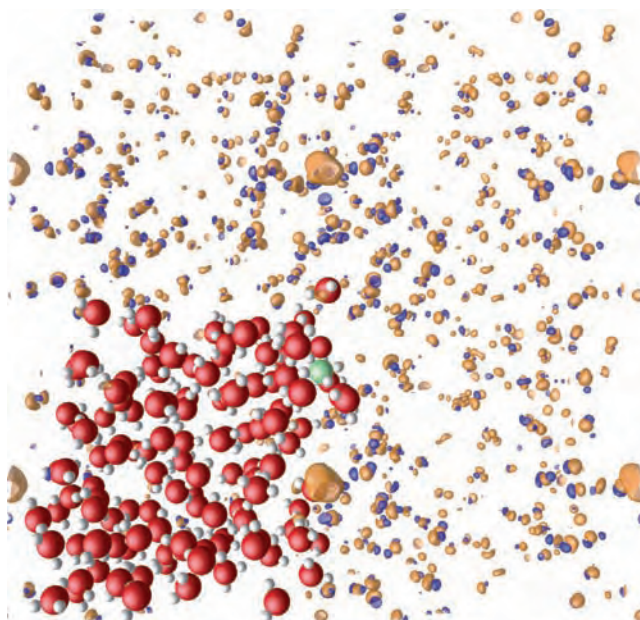
Fig. 2: *Distribution of the excess charge density of a proton in a water supercell. The extent of the charge distribution has a significant influence on the magnitude of electrostatic supercell artifacts.*

of hitherto not reported surfaces are identified (structures in Fig. 1 above the dashed line). A careful analysis showed that such conditions can be realized in experiments where the formation of H_2 molecules from chemisorbed H adatoms is slow compared to the incoming H flux. Using this concept enabled us e.g. to understand the observation of a (1×1)H adsorbate structure on ZnO(0001), which has been subject to a highly controversial debate in the literature.

The surface oxide resulting from the electrochemical reactions may protect the metal from further corrosion. Once a critical thickness is reached, the oxide layer prevents oxygen from reaching the metal or vice versa. Understanding the transport properties of the oxide layer is therefore of crucial importance. Ion transport in solid oxides occurs via vacancies or interstitials. Computational schemes for calculating the properties of such point defects have been developed for semiconductors used in (opto) electronic devices, but can be applied analogously to oxides. To render the simulation feasible, the defect is placed in a supercell with ~100 host atoms that is then repeated periodically throughout space. However, artifacts arise in supercell calculations from the periodic structure and artificially high concentrations of defects. For charged defects, the error in the defect formation energy scales asymptotically like $Q^2/\varepsilon L$, where Q is the charge, ε the dielectric constant and L the lattice constant of the supercell. We have recently developed a novel systematic scheme to correct for electrostatic artefacts in charged-defect supercell calculations [3]. The corrections are particularly important for oxides due to the comparatively low dielectric constants and large charge states that may occur. The corrections improve the accuracy of the calculated formation energies, which in turn serve as an input to the continuum description of defect distribution and migration. We are currently adapting the scheme to an aqueous environment (see Fig. 2) to improve the accuracy of calculated hydration energies that are required to establish the link between the chemical potentials and the electrochemical redox potentials.

In summary, the above examples illustrate the prospectives of first principles calculations to shed light on the corrosion process at the metal/oxide/water interface by providing accurate thermodynamic data at and on either side of the interface. In order to fully exploit the predictive power of *ab initio* calculations, new concepts and methods must be developed to map the complex environment on well-defined model systems that exhibit the key effects. This sets the stage for studying the reactions and transport processes at the atomic scale in a realistic environment. Identifying the routes and critical steps promises to reveal opportunities to block or at least slow down the corrosive process.

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Functional Adaptations of Biological Materials – Photonic Crystals in the Scales of the Beetle *Entimus imperialis* (Curculionidae)

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Controlling the optical properties of materials has become an intense research field owing to the enormous potential photonic band-structure concepts offer for all-optical information processing. One of the most essential ingredients in this field are photonic crystals, in which low-loss dielectric media with different refractive indices are periodically arranged in a volume. One central aim in this field is to obtain photonic crystals with a complete band gap at visible wavelengths, which means preventing the propagation of light with specific frequencies in all directions. So far, such structures have not been realized yet [1]. However, in nature beetles have evolved biological three-dimensional photonic crystals which operate at visible light [2-4]. Understanding their construction principle and the resulting optical properties might provide the key to open up complete photonic band gaps at visible wavelengths.

We have recently discovered three-dimensional photonic crystals inside the scales of the neotropic weevil Entimus imperialis which display a number of very interesting characteristics. Individual scales are leaf-shaped and cluster on parts of the exoskeleton (Fig. 1a, insert). Compared to previously reported findings, the scales of E. imperialis are particular in two senses. First, they can display nearly the full spectral range of visible light in each scale and second, individual colors occur in relatively large domains (Fig. 1a). Careful removal of the scale's outer shells using focused ion beam milling

(Fig. 1b-d) revealed a rod-connected photonic crystal with diamond structure. Using samples cut in different directions, we extracted dimensions and shape of the structure and reconstructed a geometrical 3D-model, which was used to confirm that all domains are formed by photonic crystals with the same geometry, but different orientations towards the shell (Fig. 1c, d). The structural parameters of the model served as input to calculate the wavelength of the reflected color for given orientations using Bragg scattering conditions, showing good accordance between calculated and observed colors (Fig. 1e).

Interestingly, transparent domains appearing in some scales (Fig. 2a, next page) were not un-structured as reported earlier [2], but contain the same structure as colored ones filled with a second solid phase (Fig. 2b), which apparently inhibits the reflection of visible light.

The composition of the scale of E. imperialis was studied by Fourier-Transform Infrared Spectroscopic Imaging. Fig. 3a (next page) shows an image in the visible spectral range. An image obtained by integrating the absorbance from transmitted light of the spectral region of the CH stretching modes (2830-3010 cm^{-1}) is displayed in Fig. 3b, while the spatial distribution of the integrated absorbance of the combined amide modes (1480-1800 cm^{-1}) is displayed in Fig. 3c. The visible image shows two domains on the beetle, separated by a "black
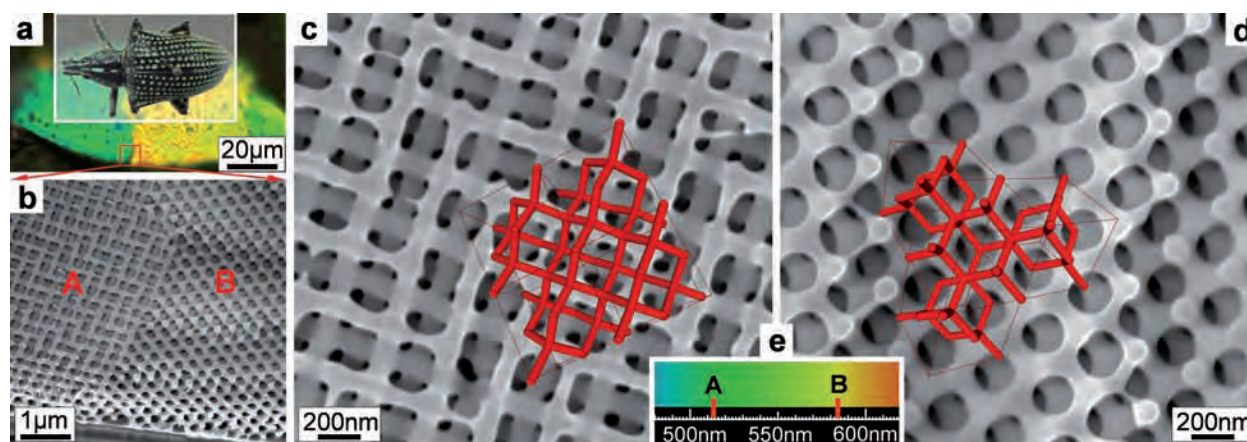
Fig. 1: *(a) Scale of Entimus imperialis (insert) showing color domains. (b) SEM micrograph of the exposed boundary between green (A) and yellow (B) domain in the polished photonic crystal. (c, d) Microstructure and 3D-model of domains A (c) and B (d). (e) Calculated color reflection for domains A and B marked in the visible spectrum.*
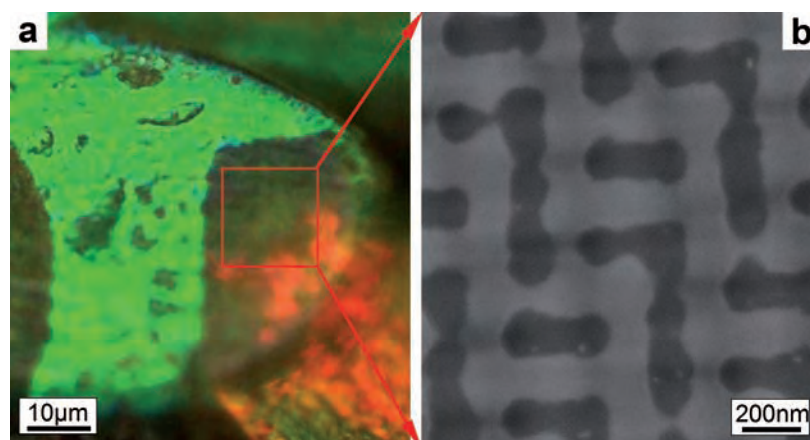
Fig. 2: *(a) Transparent domain in scale and (b) SEM micrograph of its core showing the diamond like structure with the voids filled by a second solid phase.*

line" in the middle. The contrast in the IR images shows two similar domains, which do not differ in the overall composition, but in the distribution of the respective species. While the CH distribution shows characteristic regular "spikes" in certain areas, small areas, the amide distribution shows "ribbon-like" structures.

Differences in the composition between the outer shell of the scale and the whole scale can be studied by a comparison between transmission spectra probing the overall scale and IR spectra recorded in attenuated total internal reflection (ATR) geometry, which probe only the top ~400 nm. Spectra of the CH stretching mode region are shown in Fig. 4. Here, the ratio between the peaks at 2960 cm^{-1}, usually a sign of CH_3 groups and the peak at 2930 cm^{-1}, frequently indicating CH_2 groups, is different between the two spectra, indicating differences in the material composition between outer and inner material.

In order to be able to synthesize structures with similar optical properties, further studies on the materials used to build these natural photonic crystals offers interesting perspectives.
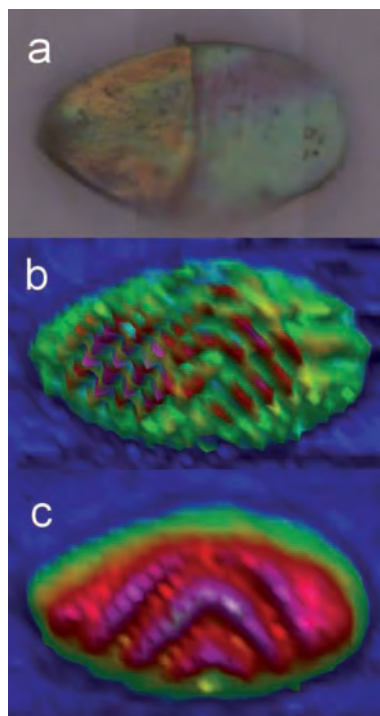
Fig. 3: *Visible (a), and two infrared images (b and c) of a single scale of E. imperialis the length of the scale was 100 μm, the width 60 μm. In the infrared images, blue colour indicates weak integral absorbance, while purple indicates strong integral absorbance.*
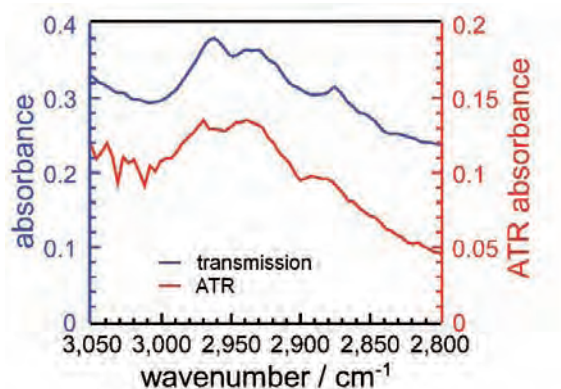
Fig. 4: *Comparision of transmission and ATR-IR spectra.*

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SELECTED HIGHLIGHTS

Ab initio Based Multiscale Simulation of Deformation Mechanisms in High-Manganese Steels

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Due to their extraordinary properties with respect to strength and formability, high-Mn steels are a material system that is intensively investigated at the MPIE and jointly with RWTH Aachen within the project SFB 761 (p. 29). Besides ongoing activities to cast and characterize the material, there has been increasing interest in a detailed theoretical analysis of their unique plasticity mechanisms. It is by now well understood that an interplay of various deformation mechanisms becomes active during mechanical loading, of which (depending on the chemical composition) the twinning induced (TWIP) and transition induced (TRIP) plasticity are the most important besides the regular lattice dislocation slip.

Both, the TWIP and TRIP effects, are associated with a change in the original ABC stacking sequence of the {111} layers in the austenitic crystal structure (Fig. 1). Therefore, the intrinsic stacking fault energy (SFE) is a decisive parameter for all mechanical simulations of the material and its accurate determination is of high relevance. Traditionally, the intrinsic SFE Γ is theoretically determined from regular and subregular solution models as

$$\Gamma_{RS} = 2\rho\, \Delta G^{\gamma\to\varepsilon} + 2\,\sigma^{\gamma\to\varepsilon}, \qquad (1)$$

where ρ is the interface atomic density. $\Delta G^{\gamma\to\varepsilon}$ labels the difference of the Gibbs free energies between the austenite (γ, fcc) and the hexagonal martensite

(ε, hcp), which is usually taken from CALPHAD databases, treating both phases at equilibrium conditions. The correction term $\sigma^{\gamma\to\varepsilon}$ is referred to as interface energy and is typically a fitting parameter since direct measurements of this energy contribution are missing. In the case of Fe-Mn-C, $\sigma^{\gamma\to\varepsilon}$ is in the range between 5 and 30 mJ/m^2, and often chosen to be 10 mJ/m^2.

A determination of the SFE without using any experimental input or fitting parameters is possible, if *ab initio* approaches such as density functional theory are used [1,2]. From the different approaches to do this, the Axial Next Nearest Neighbour Ising (ANNNI) method is computationally the most efficient choice, as it reduces the calculations to a series expansion of defect free supercells. In first order the intrinsic SFE is given as

$$\Gamma_{ANNNI} = 2\rho\, (G\,[AB]\text{-}G\,[ABC]). \qquad (2)$$

The main difference compared to Eq. (1) is the choice of the Gibbs free energies. Whereas in Eq. (1) the ground state free energies of the bulk phases enter, an *ab initio* evaluation of Eq. (2) provides the unique opportunity to directly simulate the actual experimental configuration (Fig. 1), namely, the formation of the stacking fault in between two Shockley partials. In this situation, the resulting ε martensite is constrained both with respect to lattice constants and to the magnetic reconstruction by the surrounding γ lattice. Comparison of both strategies yields the interface energy term

$$\sigma^{\gamma\to\varepsilon} = \rho\, (G\,[AB]\text{-}G\,[ABC] - \Delta G^{\gamma\to\varepsilon}). \qquad (3)$$

While at first glance this may look like a formal mathematical transformation, we could demonstrate that $\sigma^{\gamma\to\varepsilon}$ can be predicted in DFT with an accuracy that is roughly one order of magnitude more accurate than the absolute SFE providing a hitherto not achievable predictive power.

For a chemically disordered binary Fe-Mn alloy, the results are presented in Figs. 2 and 3 considering two magnetic structures, where the paramagnetic version is closest to reality. The SFE changes in both cases strongly with increasing Mn content. As shown in Fig. 2, a minimum of the SFE occurs for the paramagnetic structure at intermediate Mn contents, in qua-
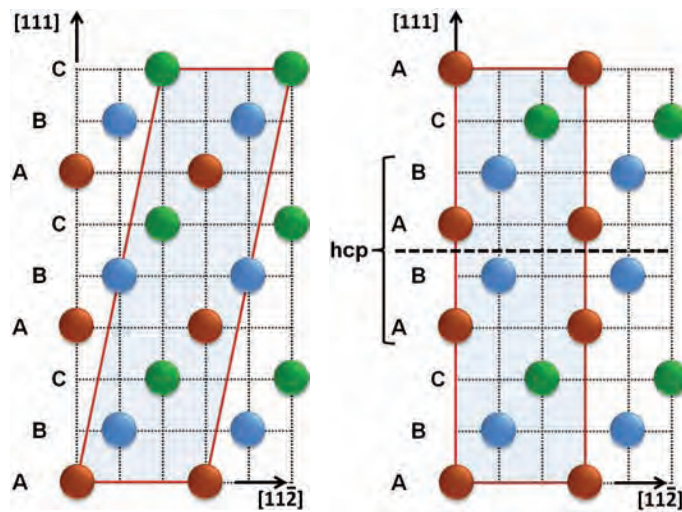
Fig. 1: *Stacking sequence of {111} layers of undisturbed austenite (left) and austenite containing an intrinsic stacking fault (right). The different coloring of the atoms indicates the stacking of the layers. The shaded area visualizes the supercell used in explicit DFT calculations.*
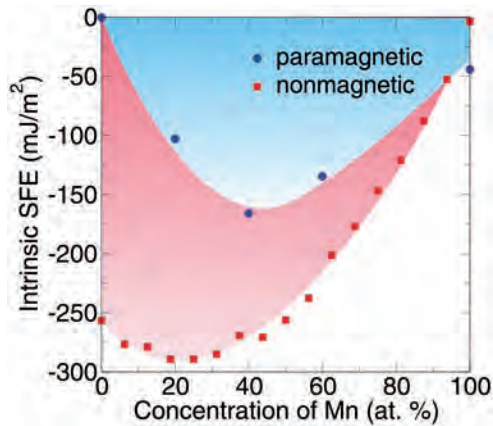
Fig. 2: *Ab initio determined dependence of the SFE on the Mn content in a chemically disordered binary Fe-Mn alloy for two different magnetic configurations. The results are aligned to the paramagnetic result for pure Fe.*

Fig. 3: *Ab initio determined dependence of the interface energy $\sigma^{\gamma \to \varepsilon}$ on the Mn content. The result for two different magnetic configuratons, as well as the empirical chosen value of 10 mJ/m² for Fe-Mn is shown.*

litative agreement with experimental findings. Using these *ab initio* results we are now in the position to inspect $\sigma^{\gamma \to \varepsilon}$, particularly whether it is indeed constant as commonly assumed. While this is roughly the case for the unphysical situation of non-magnetic calculations, including paramagnetism results in a strong nonlinear dependence of the interface energy with Mn content (Fig. 3). The "divide and conquer" strategy, discussed here, decomposes an engineering quantity (here: the SFE Γ) into contributions, which are readily and with high accuracy available by empirical and experimental methods (here: CALPHAD Gibbs free energies $\Delta G^{\gamma \to \varepsilon}$) and contributions not accessible by experiment, but which can be accurately computed employing *ab initio* techniques (here: interface energy $\sigma^{\gamma \to \varepsilon}$). It implies a paradigm change from a full-field *ab initio* approach, but will likely have a big impact on rendering *ab initio* predictions useful for more complex engineering problems.

Such obtained insights for the SFE have subsequently been used in constitutive models that are based on lattice-defect rate formulations to predict the strain-hardening. Motivated by experimental characterizations of high-Mn steels, the volume fraction of twins as well as the dislocation structure and their respective deformation-driven evolution are taken into account. The chosen approach differs from previous models such that only physically motivated parameters with crisp upper and lower bounds are used to describe the processes related to the twinning of materials. A key parameter entering the equation for the critical stress of twin formation

$$\tau_c^\beta = \frac{\Gamma}{3b^\beta} + \frac{3\mu b^\beta}{L_0} \qquad (4)$$

is the stacking fault energy. The other symbols are the shear modulus μ, the Shockley partial Burgers vector b^β and the line length of an immobile Shockley partial L_0 [3]. After fitting the phenomenological parameters of the rate model within admissible bounds the model can then be used to predict the macroscopic strain-hardening behavior of TWIP materials (Fig. 4). Using a consistent set of parameters, an excellent agreement of the derived curves with experimental data from compression tests of a Fe-23%Mn-0.6%C steel is obtained. The results demonstrate the novelty and power of the chosen *ab initio* based multiscale approach in crystal plasticity, as matching the hardening behavior is much more difficult than fitting the stress-strain curve itself.

Fig. 4: *Influence of temperature on the strain-hardening behavior of Fe-Mn alloys. The strain hardening curves for different temperatures are compared to experimental data. The multiscale simulations are based on lattice defect rate formulations in conjunction with kinetic equations of state and SFE data that are obtained directly by ab initio predictions. The same set of physical parameters is used for all temperatures.*

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The Magnetism of Iron Based Materials:
A First-Principles Derivation of Thermodynamic Properties

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An accurate prediction of the Gibbs free energy is the basis to compute phase diagrams, finite temperature materials parameters, or kinetic barriers, and is thus fundamental in materials design. The most challenging contributions - but crucial for many structural materials - are related to the magnetic degrees of freedom [1]. We have recently shown their high relevance, when considering martensitic phase transitions in the magnetic shape memory alloy Ni_2MnGa. For this system, we revealed that the excitation of spin waves dramatically affects the dynamic stability of the austenite phase [2]. Only taking this mechanism into account, we were able to describe the martensitic phase transition correctly.

For iron-based materials, the Heisenberg model has proven to yield a numerically efficient yet sufficiently accurate description of magnetic excitations. It provides an elegant way to couple ground state *ab initio* calculations, which are used to determine the exchange integrals, with concepts of many-body theory to describe the full temperature dependence of excited magnetic states and to predict critical temperatures [3]. To use this concept for realistic materials we implemented and carefully checked a number of analytical and numerical approaches with respect to numerical efficiency and predictive power. In this context, the specific heat capacity C_p has been identified as a critical quantity, which provides also a close link to experiments and in addition to empirical CALPHAD simulations.

Our analytical approach to the free energy of the Heisenberg spin system [4], which is based on the random phase approximation, in combination with vibronic (quasiharmonic approximation) and electronic (finite temperature DFT) contributions, allowed us to obtain a remarkably accurate description of C_p below the critical temperature (see Fig. 1a). For a proper description of the region above the critical temperature, however, short range correlations are critical and need to be taken into account. We therefore explored various Monte Carlo (MC) schemes. Classical MC calculations that neglect quantum effects, yields significant short comings in the low temperature regime (see purple area in Fig. 1a). We have, therefore, derived from an extensive set of quantum and classical Heisenberg model systems a rescaling scheme [5], which provides the accuracy of QMC calculations at much cheaper numerical costs. Analyzing this concept in more detail, we discovered a universal behavior of the thermodynamic properties for the Heisenberg model with respect to the kind of the interaction (long- vs. short-ranged, ferro- vs. anti-ferromagnetic) and the lattice structure.

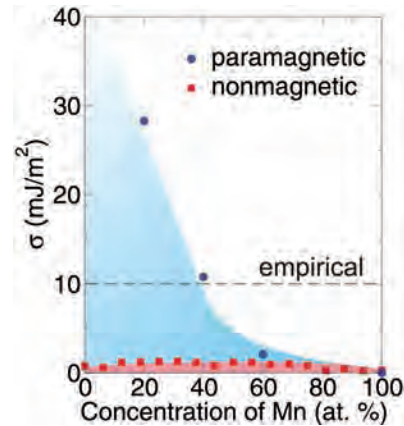This universality motivates the definition of an effective nearest-neighbor Heisenberg model with just one interaction parameter. The latter is, e.g., related to T_C, which can be either determined by *ab initio* calculations [3] or taken from experiment. Treating this effective model with QMC yields for bcc
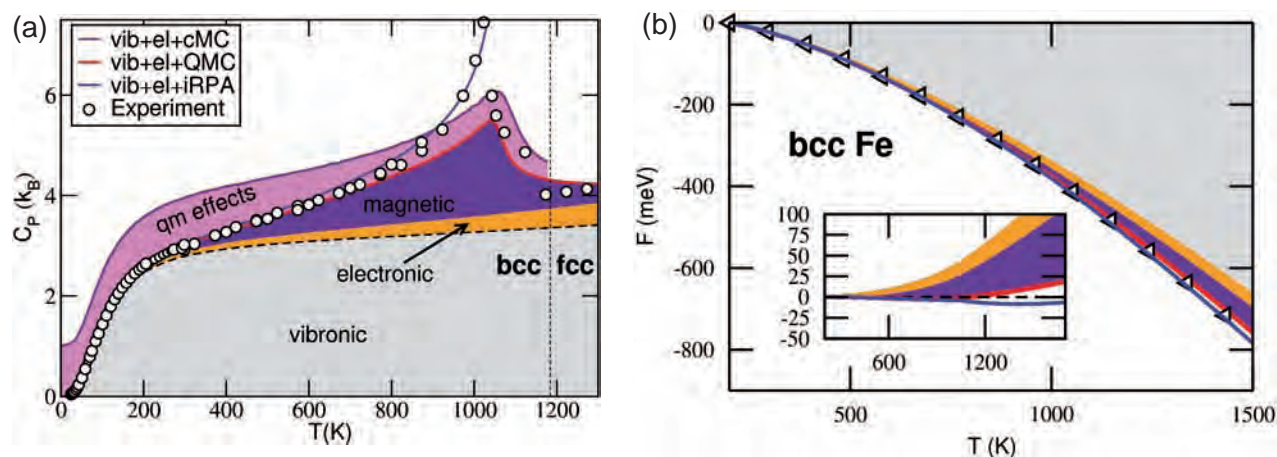
Fig. 1: *Derivation of (a) the specific heat capacity and (b) the free energy of bcc iron, including magnetic, electronic and vibronic contributions. The results for all three theoretical approaches described in the text are shown and compared with CALPHAD (triangles) and experimental data (circles) [3,4].*
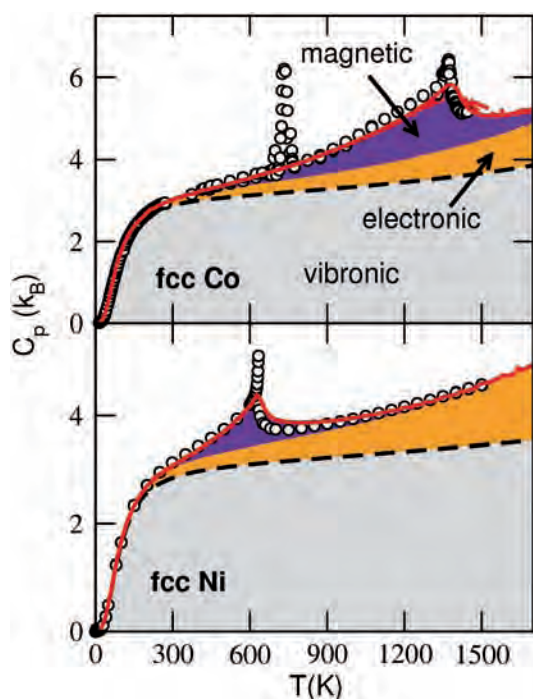
Fig. 2: *Calculated specific heat capacity (red line) for fcc Co and Ni as compared to experiment (circles). For the magnetic contribution to the free energy the QMC data for the effective Heisenberg model are used [6].*

Fe an excellent agreement with experimental $C_p(T)$ data and free energies (Fig. 1). The application of the same approach to the 3d ferromagnets cobalt and nickel (see Fig. 2), demonstrates its excellent transferability to other magnetic systems containing a single magnetic species [6]. We have, therefore, applied the developed methodology to more complex systems, such as, e.g., cementite (Fe_3C), which is a highly relevant phase for steel design. Due to a large scatter in the experimental C_p (see Fig. 3a)

an unambiguous thermodynamic assessment (e.g., CALPHAD) of this system is challenging. As demonstrated in Fig. 3, our method yields not only a clear prediction of $C_p(T)$ particularly in the high temperature regime [7], it also provides a hitherto not achieved insight into the impact of magnetic contributions to the phase stability of Fe_3C (Fig. 3b) [8].

In conclusion, the set of *ab initio* based methodologies developed in the last years allows a reliable and parameter-free prediction of the magnetic contribution to the free energy of materials, a systematic separation from other physically relevant contributions to the thermodynamic properties, and can be applied to a wide range of materials.

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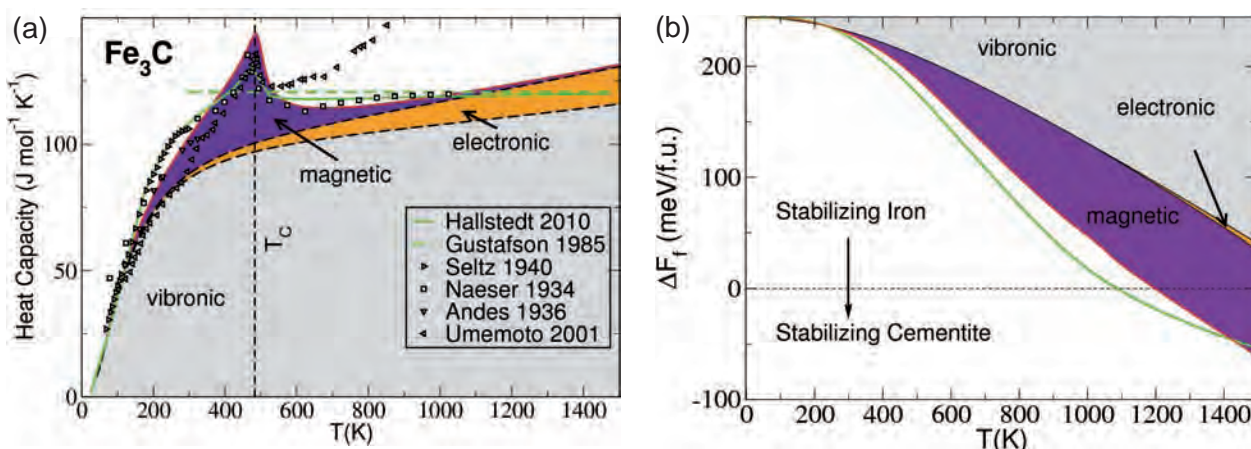
Fig. 3: *Different ab initio determined contributions to (a) the specific heat capacity and (b) the formation enthalpy of cementite [6,7]. The latter is aligned with CALPHAD at T = 0 K. Our theoretical approach is compared to experimental data (black symbols) as well as two CALPHAD assessments (green lines).*

Quantum-Mechanical Approaches to the Elasticity of Complex Alloys

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The vast majority of commercial metal-based products are alloys. For these multi-component and often also poly-grain and multi-phase materials mechanical properties are among the most important characteristics. Centuries of metallurgical efforts have resulted in a broad spectrum of different materials with either versatile applications or highly specialized uses in the form of specific *niche* products. Recent progress in new technologies substantially increased the need for an accelerated design of new application-tailored and highly specific metallic alloys. Theory-guided materials design offers a promising and powerful approach in this context ideally complementing experimental synthesis, processing, and characterization techniques.

Modern theory-guided materials design is a bottom-up multi-scale strategy where quantum-mechanical electronic-structure calculations are applied at the atomic level to rapidly screen a vast amount of possible chemical compositions with respect to desired structures and properties. Focusing for example on elastic properties, once the compositional trends of single-crystalline elastic constants have been determined, numerically-robust homogenization techniques [1-3] are employed to predict macroscopic elastic moduli for polycrystalline alloys as occurring in real products. Using this approach both atomic- and macro-scale elasticity can be systematically examined and the most promising alloy candidates are theoretically pre-selected in order to minimize the duration as well as costs

of subsequent experimental casting and testing steps. For example, fundamental materials design limitations preventing a simultaneous increase of both ductility (measured by the bulk over shear modulus ratio B/G) and stiffness (specific Young's modulus Y/ρ) in single-phase materials could be identified (see Fig. 1) in body-centered cubic (bcc) Mg-Li alloys [4,5]. Even when going from binaries to ternaries (MgLi-X) this limitation could not been overcome.

In order to achieve such critical insight into materials behaviour and chemical trends, efficient and accurate theoretical tools are required for the prediction of alloy elasticity. The elastic constants of pure phases can nowadays be routinely calculated (even above 0 K) using electronic structure methods. In contrast, the prediction of the elastic properties of low-symmetry systems such as random alloys is less straight forward. In particular, the faithful reproduction of randomness in these structures poses a major challenge as it is not compatible with the widely-implemented concept of periodic boundary conditions applied to rather small computational cells forming thus infinite defect-free single-crystals.

A *naïve* atomistic description of disordered alloys based on a randomly generated atomic distribution requires a huge configuration space and can hence only be achieved using large supercells, which render standard electronic structure methods unfeasible. Instead three alternative approximations are generally employed: the coherent potential approximation (CPA,
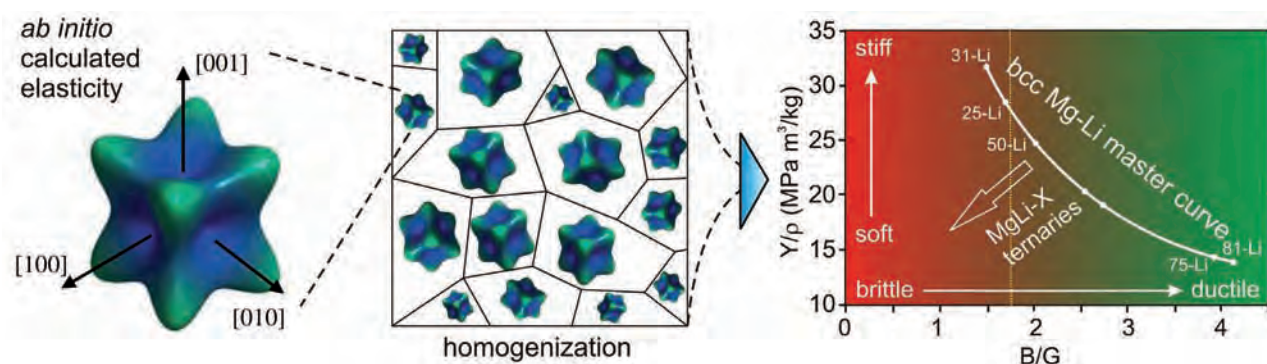
Fig. 1: *Schematic representation of theory-guided materials design. Its effectiveness is illustrated on the identification of fundamental materials design limits in the bcc Mg-Li alloys [4,5].*
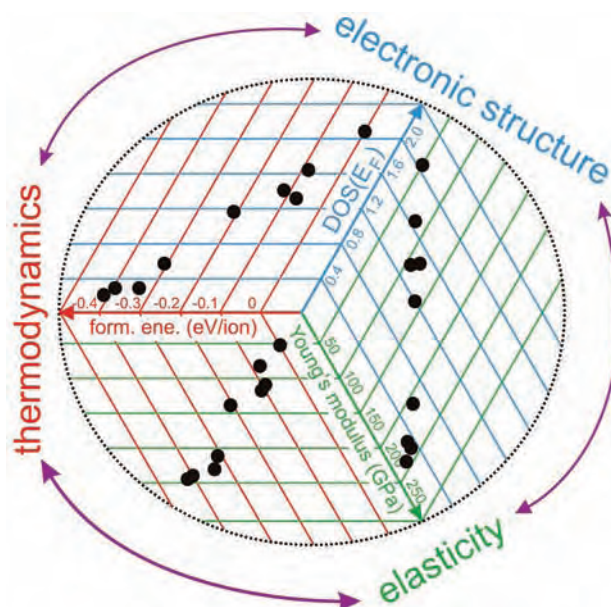
Fig. 2: *Mutual correlations (manifesting themselves as nearly linear trends) between the formation energy, Young's modulus and density of states at the Fermi level identified by quantum-mechanical calculations in bcc Fe-Ti alloys.*

We have recently shown for the example of two-phase Fe-Ti alloys that the *ab initio* guided design can be extended to multi-phase materials. Combining thermodynamic considerations with studying the elasticity of various single- and poly-crystalline Fe-Ti alloys, the origin of ductility and softness of one of the Fe-Ti phases (β-Ti(Fe)), and stiffness of the other (intermetallic FeTi) could be explained. It became further possible to link this insight to our previous results on Ti-Nb alloys [12] and identify very strong correlations between the three fundamental materials characteristics (see Fig. 2): (i) atomistic-level electronic structure (specifically the density of states at the Fermi level), (ii) thermodynamic stability (quantified by the formation energy), and (iii) macroscopic polycrystalline elasticity (characterized by the value of Young's modulus).

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see e.g. [6,7]), the cluster expansion (CE) method [8,9] and special quasi-random structures (SQSs, for details see [10]). In case of tensorial properties, as e.g. the anisotropic elasticity, the SQS approach offers interesting advantages since it is computationally not demanding yet allows the inclusion of local relaxation effects. Recently, we have therefore generated a set of system-independent 32-atom SQS spanning the entire concentration range and used it to determine elastic constants of face-centered cubic (fcc) binary alloys [11]. The performance of this approach was tested by comparing with fully converged 4000-atom supercells. Due to the fact that computational effort for standard *ab initio* techniques increases with the second or third power of the number of atoms, the SQS approach allows to reduce computational times by four to six orders of magnitude compared to a direct brute force approach without loosing accuracy.

Ab initio Growth Simulations of Crystalline Nanostructures

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Nanotechnology has evolved over the last decade to one of the major key technologies in materials science: The physics and the properties of materials can be tremendously altered if the size of the system is reduced below a critical length associated with these properties. Being able to design and control chemical composition, size, and/or shape of the nanostructures open new opportunities in a wide range of technologies: catalysis, hydrogen storage, biotechnology, sensorics, micro- and nano-electronic are only few fields where new applications are emerging [1-5].

We have recently developed a hierarchical set of tools to study the time evolution of nanowires starting from fundamental atomistic growth mechanisms. In this brief report we highlight the power and the insight such an approach allows. As prototype example we consider GaN nanowires (NWs). GaN NWs constitute an interesting system for investigation due to their unique and peculiar growth mechanisms: In contrast to Vapor-Liquid-Solid (VLS) catalyst assisted growth for non-nitride III-V NWs, GaN based NWs can be self-assembled. This finding suggests that the growth mechanism in GaN NWs is substantially different from the well understood VLS growth of traditional III-V NWs. A detailed understanding of the very different and technologically highly relevant growth behavior is therefore

In order to gather a complete and consistent description of the growth of these NWs we had to take into account (i) the surface morphologies of the side facets and the top surface at the experimentally relevant growth conditions, (ii) the material transfer through surface adatom diffusion from the substrate to the side facets and to the top surface, and (iii) the experimentally relevant growth geometries. The latter may lead to shading effects as well as to Ga and N adatom spatial separation. In order to incorporate the aforementioned effects which span the atomistic up to the experimentally relevant length scales and provide a consistent description of the growth of GaN NWs we have developed an integrated approach that describes all aspects of material transport on the mesoscopic scale. All input parameters entering this model have been computed based on *ab initio* derived surface phase diagrams and subsequent analysis of the adatom diffusion paths.

In order to obtain the thermodynamic and the kinetic parameters for the relevant a- and m-plane GaN surfaces we performed plane wave pseudopotential calculations within density functional theory. Our calculations revealed that m-plane surfaces are energetically most favorable for the experimentally relevant growth conditions (high N over Ga ratio of partial pressures and high growth temperatures). Based on the calculated surface structures we have determined the potential energy surface for a Ga and a N adatom on them [6]. The energy surfaces revealed a wealth of hitherto not identified phenomena. For the Ga adatoms a strong anisotropy in the diffusion barriers for both a- and m-plane surfaces was calculated. For the m(a) plane surface larger diffusion barriers are found for diffusion along (normal to) the c-axis (the axis of the NW) (see Fig. 1(b)). With respect to N adatom diffusion our results show qualitatively different adatom kinetics: Placing a N adatom close to a surface N atom, it attracts the N surface atom, forms a strong N-N bond, and desorbs together with a surface N atom as a N molecule.

Based on a careful analysis and calculation of all the atomistic growth events we could identify the key processes. For example: The surface thermodynamics and adsorption kinetics reveal that for the N-rich experimentally relevant growth conditions the side facets of the NWs are stoichiometric and intrinsically unstable to atomic N. This is in contrast to the thermodynamically stable surface morphologies of the top surface [7]. Hence, nucleation events (which require the presence of both species at neighboring positions at the same time) and subsequently incorporation rates should be lower in the side facets.

Based on this insight and using the *ab initio* computed kinetic parameters we were able to construct a quantitative mesoscale growth model (Fig. 1(c)). The equation which describes the time evolution of the adatom density spatial distribution is the following:

$$\frac{d\rho(\boldsymbol{r},t)}{dt} = \Phi_{imp} + D\nabla^2\rho(\boldsymbol{r},t) - \frac{1}{\tau_{des}}\rho(\boldsymbol{r},t) - \frac{1}{\tau_{inc}}\rho(\boldsymbol{r},t)$$

where, $\rho(\boldsymbol{r},t)$ is the adatom density at position $\boldsymbol{r}$ and time t, Φ_{imp} is the impinging flux, and τ_{des}^{-1}, τ_{inc}^{-1} are
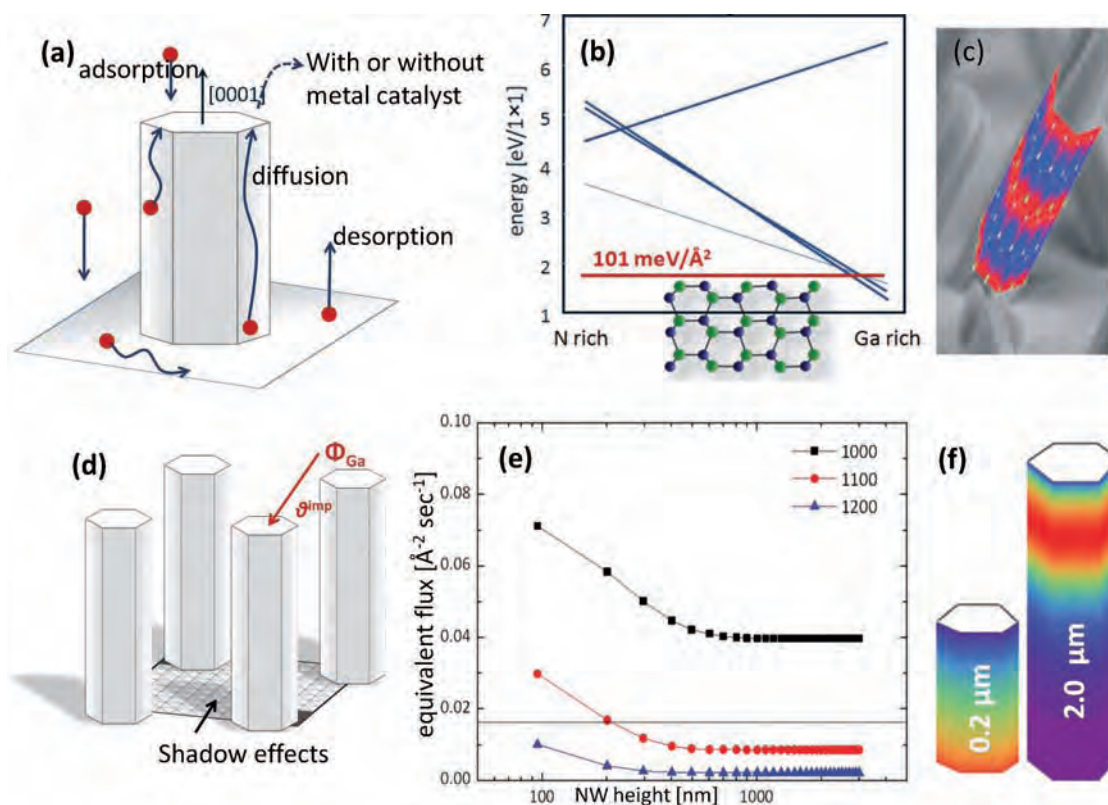
Fig. 1: *(a) Schematic representation of the atomistic mechanisms occurring during the epitaxial growth of NWs. (b) Surface thermodynamics (c) schematic representation of the potential energy surface for the adatom diffusion on the side facets. (d) Illustration of the geometry used to model an array of NWs. (e) Ga adatom flux at the top of the side facet for various NW heights and various experimentally relevant temperatures. (f) Ga adatom density distributions at T = 1000 K and NW heights 0.2 and 2 µm respectively.*

the desorption and incorporation rates respectively. In our model we assume steady state conditions ($d\rho/dt = 0$) and negligible incorporation rate in the side facets ($\tau_{inc} = 0$).

Using our mesoscale model we were able to describe/explain a large variety of growth conditions. These studies revealed that for the relevant growth temperature window the desorption limited axial diffusion length for the is smaller than 200 nm. Furthermore, they revealed that the adatom flux shows an inverse exponential dependence on the temperature. However, the aforementioned flux decreases with the height of the NWs and converges (to different values for the different growth temperatures assumed) for NW heights larger than 0.5 µm. This is due to (i) shading effects which become important for longer NWs and (ii) the limited diffusion length. While the diffusion length is a temperature dependent material parameter, shading effects are based solely on geometric parameters and they may thus be controlled, e.g. by patterned nano-lithography.

In summary we have developed an *ab initio* based hierarchical approach to investigate the growth of crystalline nanowires. Our approach incorporates realistic growth geometries and conditions and provides a full qualitative and even quantitative

description. The approach has been successfully employed to predict the growth rate of the NWs as function of the growth parameters (e.g. parameters that can be fully controlled experimentally). The hierarchical growth model developed here can be easily generalized to other material systems and nanostructures.

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Scanning Electrochemical Potential Microscopy (SECPM): Numerical Investigation and Applicability

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High resolution measurements of the lateral and vertical electrode potential distribution at the electrode/electrolyte interface are of interest in many research fields from galvanic elements in corrosion to electrochemically active sites in biological cells. The scanning electrochemical potential microscopy (SECPM) was designed for such measurements in electrolytes [1]. In view of experimental results contradicting the Gouy-Chapman-Stern theory [1], we investigated the applicability of this new scanning probe technique in resolving the electric double layer (EDL) vertical potential profile at the electrode/ electrolyte interface [1,2]. Our main objective was to develop a description of the measurement mechanisms and to investigate the effects of the probe and its EDL in such an experimental configuration.

Within the framework of the modified Poisson-Boltzmann equation, a finite element simulation of the SECPM has been carried out. A typical geometry of the probe near the electrode surface is shown in Fig. 1. We studied the effect of the metallic protrusion geometry and suggested the use of a flattened metallic protrusion for best reproduction of the vertical potential profile near the electrode [3]. Even if the EDL Debye length is significantly greater than the metallic protrusion height, a sharp metallic protrusion generates a highly non-uniform distribution of the surface charge density distorting
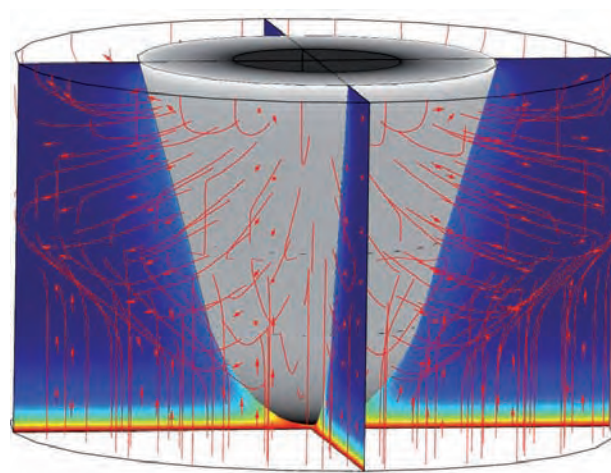
Fig. 1:. *Distribution of the potential and the electric field inside the electrolyte and the coated probe for an electrode potential of 100 mV. The red arrows show the orientation of the electric field in the electrolyte domain.*

the EDL. Furthermore, the overlap effect of the probe and electrode EDLs has been studied by considering different EDL polarities and strengths. The overlap was analyzed in terms of potential and ion distributions in the separating gap. We observed that the obtained SECPM potential profiles are a direct consequence of the EDLs overlap [3]. Depending on the strength and the polarity of both
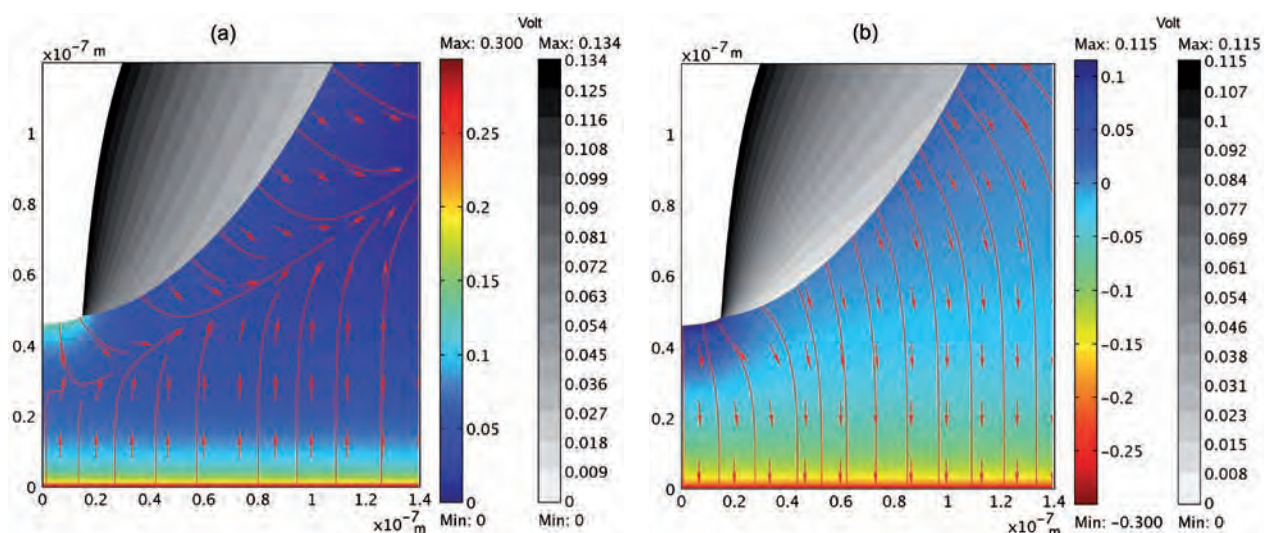
Fig. 2: *Potential distribution and electric filed lines in the probe/electrode gap for positive (a) and negative (b) applied potential (±300 mV). The red arrows represent the orientation of the electric field lines.*
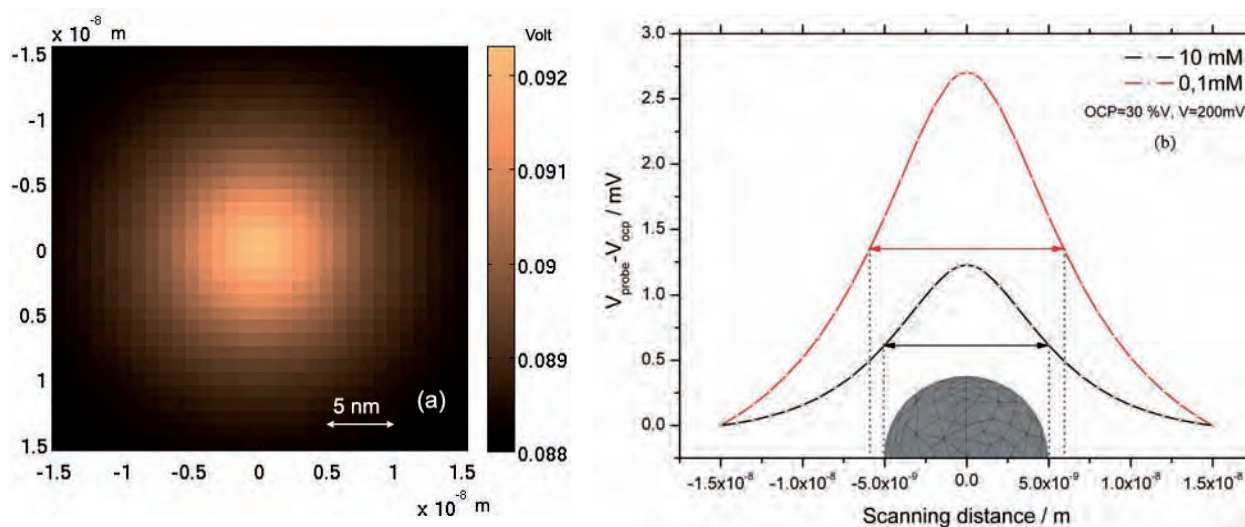
Fig. 3: *(a) 2D image of the nano-hemispherical particle obtained by simulating a 2D SECPM scan. (b) Corresponding scan line over the nano-particle for two different electrolyte concentrations.*

EDLs, the probe potential is severely affected by Debye screening, which is illustrated in Fig. 2. The observed screening effect and the overlap of the EDLs from probe and electrode lead to the conclusion that the EDL potential profiling by SECPM is not a straightforward measurement, and complex data analysis is needed to extract the unperturbed EDL potential from the measured profile [3].

The SECPM has a second operating mode in which the probe is scanning in xy directions parallel to the electrode providing a surface electrode potential mapping [4]. Simulations of 2D scans have been carried out for a hemispherical nano-particle deposited on the electrode surface. A simulated image of the particle is displayed in Fig. 3a. As it is the case for most SPM techniques, the SECPM probe apex has a dominant effect on the observed size of the imaged particle [5]. In contrast to the profiling mode, the probe apex has to be as sharp as possible in order to ensure a good lateral resolution of the SECPM image, even though at the same time the accuracy of the potential values is compromised. Besides, the apparent size of the imaged particle crucially depends on the electrolyte concentration: the apparent size decreases with increasing electrolyte concentration, which corresponds to a decrease of the EDL Debye length and hence the iso-potential planes in the EDL are more compact and closer to the electrode surface. This behavior can be seen in the lateral potential profiles of Fig. 3b. On the other hand, higher electrolyte concentrations increase the Debye screening, leading to lower overall sensitivity of the probe [5]. Optimum sensitivity is achieved at opposite probe/sample EDL polarities. Our results qualitatively explain the differences in size of the imaged particles observed by comparing images obtained using SECPM and electrochemical STM [4].

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Atomistic Investigation of Selective Dissolution

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In alloy systems, dealloying is a corrosive process owing to different electrochemical activities of alloy components [1]. Normally, this corrosion process is detrimental and it has been pointed out to be the cause for perilous material deterioration, e.g., stress corrosion cracking of stainless steels. Historically, the process was used by goldsmiths in ancient times, which was termed as Depletion Gliding (Fig. 1a) or 'Mise en Couleur'. The process involves removal of base metals from the surface layers of a cheaper alloy to leave them considerably enriched in precious metal. In a binary alloy, selective dissolution of less noble component in a corrosive environment often results in a porous network of nobler alloy. Porous materials comprises of a solid skeleton interspersed with pores or voids. Such architecture provides a material with high specific surface area and low specific weight, which qualify them for many applications as catalysts, sensors, and actuators. Today, selective dissolution is being utilized to produce materials of potential technological importance, for instance, the most active catalyst particles for the oxygen reduction in fuel cells.
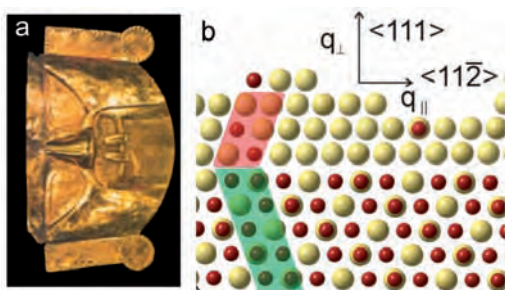
Fig. 1: *a) Pre-Columbian mask (Peru) prepared by depletion gilding. b) Stacking reversed ultra-thin film observed during the initial stages of selective dissolution of $Cu_3Au(111)$.*

The simplest scenario of dealloying occurs, if a binary alloy of elements with sufficiently different Nernst potentials is exposed to an aqueous electrolyte in which no stable bulk oxide is formed. The fundamental understanding of the selective dissolution process has been largely studied using noble metal binary alloys like Cu-Au. Cu dissolves initially as the surface is polarized above the corresponding equilibrium potential, E_{eq} [1]. Beyond a so-called critical potential E_c, and with a sufficiently high content of the more reactive element in the alloy
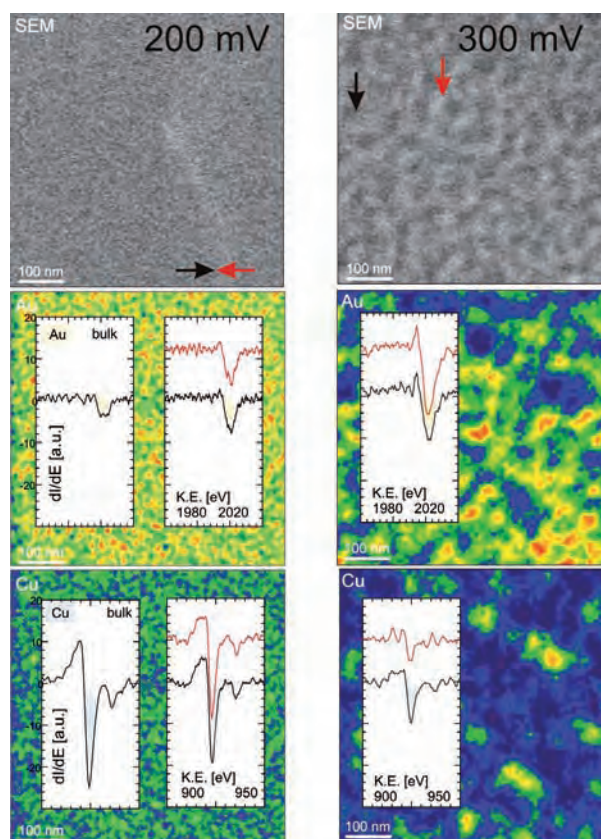
Fig. 2: *Scanning Auger Microscopy images with a resolution below 10 nm on surfaces after 1h of dissolution at 200 mV (left) and 300 mV (right) . Point scans show enrichment in Au at surface.*

(i.e. parting limit), the entire alloy then transforms into the mentioned nanoporous network of the noble element. Our previous in-situ X-ray diffraction results [2-4] showed that upon increasing potential above E_{eq}, an epitaxial ultra-thin Au-rich passive layer forms with inverted stacking sequence than that of the substrate (Fig. 1b). Inverted Au islands then grow at medium overpotentials (~ 300-400 mV). The observation of a stacking reversal in the surface film indicates that the Au atoms arrange themselves in an energetically favourable orientation probably via surface diffusion.

So far it was not clear if these Au film covers the entire surface at that stage. Therefore we carried out scanning Auger microscopy (SAM) measurements to analyze the chemical composition of the dealloyed Cu_3Au (111) surface. Figure 2 shows the scanning Auger maps and SEM images of the Cu_3Au (111)
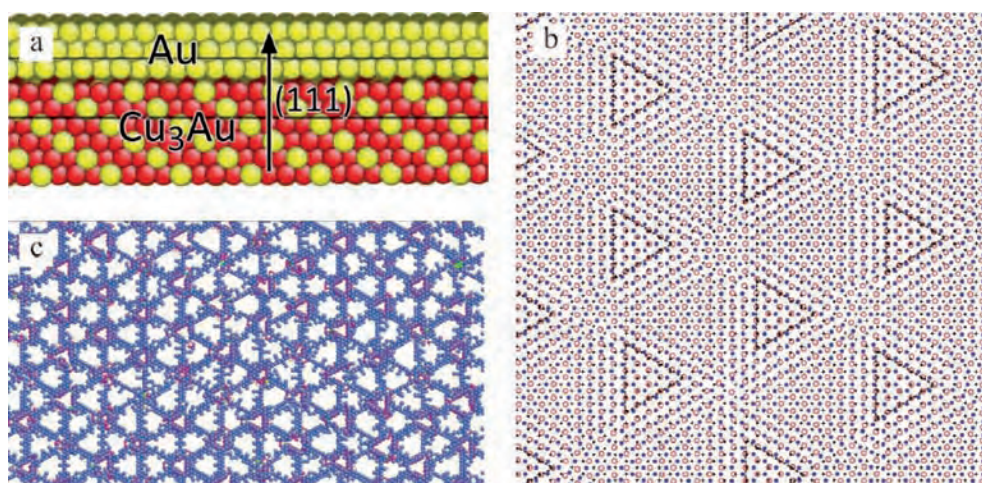
Fig. 3: *Atomistic simulations of an ultrathin (3 ML) Au film on a Cu_3Au (111) substrate. The calculations show the formation of a triangular network of misfit dislocations.*

surface dealloyed at 200 and 300 mV, respectively. At 200 mV, initial stripping of Cu from the alloy surface already results in Au-rich alloy surface. Quantitative analysis provided a thickness of Au of 1 monolayer. At 300 mV, further dissolution of Cu leads to the formation of Au islands, which is evident from the scanning Auger maps. Also between the islands the surface is enriched in Au. After removing the dealloyed surface (sputtering) we recover the original composition of Cu_3Au (111).

At the interface between the Au layer and the Cu-Au substrate the local coordination across the interface is modulated including very unfavourable positions. In order to gather a deeper and on-atomic-scale understanding of the strain relaxation mechanisms underlying the Cu_3Au/Au system we performed large scale calculations using Embedded Atom Method (EAM) potentials [4]. For the interatomic interactions of the Cu-Au alloy system the parametrization proposed by Barrera et al. is used [5]. We performed the atomistic simulations of an ultrathin (3 ML) Au film on a Cu_3Au (111) substrate. We modelled the Cu_3Au/Au (111) surface using a slab geometry consisting of 6 monolayers (MLs) of Cu_3Au in the $L1_2$ crystal structure and 3 MLs of a Au adlayer (see Fig. 3a). The Au adlayer is by 5% biaxially compressed while the Cu_3Au substrate is strain free. The atomic positions of the top 6 MLs are relaxed by a simulated annealing procedure while the bottom 3 MLs of Cu_3Au are kept fixed.

Our calculations revealed that the in-plane strain of the Au adlayer is accommodated by the formation of a triangular network of misfit dislocations which separate regions of fcc and hcp stacking sequences. These regions are shown in Fig. 3b and have a triangular shape and are laterally arranged in a

hexagonal pattern. The aforementioned disregistry network is clearly illustrated in Fig. 3c where only the atoms which deviate from the ideal fcc 12 times coordination are shown. This network has an average thickness of 3 MLs and extends by 2 MLs in the Cu_3Au substrate. The underlying local strain along the modulated surface layers should also favour the exchange of atoms between the interface and surface layers even at room temperature, although dislocation networks were not observed sofar for the initial dealloying of Cu_3Au (111). One may speculate that if we have interdiffusion from the substrate to the adlayer this may preferentially occur in the disregistry regions.

The influence of the strain at the substrate-overlayer interface is expected to be large especially during the initial formation of the (flat) thin passive layer in the regime below the critical potential. A detailed comparative study between Cu_3Au and e.g. the nearly strain-free system Ag-Au has not been reported to date.

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PART IV.

GENERAL INFORMATION AND STATISTICS

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NEUGEBAUER, Jörg, Prof. Dr. rer. nat. (since Nov. 2004)
RAABE, Dierk, Prof. Dr.-Ing. (since July 1999) *
STRATMANN, Martin, Prof. Dr. rer. nat. (since Jan. 2000) **

* chief executive since Sep. 29, 2010
** chief executive until Sep. 28, 2010

Emeriti:
NEUMANN, Peter, Prof. Dr. rer. nat.
PAWELKSKI, Oskar, Prof. Dr.-Ing.
PITSCH, Wolfgang, Prof. Dr. rer. nat.

Max Planck Fellow:
EGGELER, Gunther, Prof. Dr.-Ing. (Ruhr-Universität Bochum, since May 2010)

External Scientific Member:
HILLERT, Mats, Prof. Dr., Stockholm, Sweden
KIRCHHEIM, Reiner, Prof. Dr., Göttingen (since April 2010)

Guest Scientists

Computational Materials Design

Kioseoglou, Joseph, Dr. (Greece) 2010-06-20 to 2010-07-20, Exchange Program Aristotle University, Thessaloniki/Greece

Okatov, Sergey, Dr. (Russia) 2010-04-12 to 2010-05-10, CJSC Institute Ekaterinburg/Russia, MPS Research Scholarship

Rayson, Mark, Ph.D. (UK) 2008-05-01 to 2009-12-31, Scholarship Alexander-von-Humboldt-Stiftung

Van de Walle, Chris G., Prof. (USA) 2010-06-12 to 2010-07-11, Materials Department, University of California, Santa Barbara/USA, Humboldt Research Awardee

Vsianskà, Monika, M.Sc. (Czech Republic) 2010-01-11 to 2010-01-30, Masaryk University, Brno/CZ, COST, European Cooperation in Science and Technology

Interface Chemistry and Surface Engineering

Deb, Pritam, Prof. (India) 2009-08-1 to 2009-08-31 and 2010-07-01 to 2010-08-31, Tezpur University, Napaam Tezpur, India, Max Planck India Fellow

Izzuddin, Hubby, M.Sc. (Indonesia) 2010-05-15 to 2010-12-31, Research Center for Physics, Indonesian Institute of Sciences, German Academic Exchange Service (DAAD)

Kawano, Takashi, Dr. (Japan) 2008-11-01 to 2010-10-31, Steel Research Laboratory, JFE Steel Corporation

Liu, Huachu, M.Sc. (China) 2010-10-01 to 2011-09-30, School of Material Science and Engineering, Shanghai University, China, State Scholar Fund of China

Prabhudev, Sagar (India) 2010-05-03 to 2010-07-31, National Institute of Technology Surathkal, India, German Academic Exchange Service (DAAD)

Microstructure Physics and Metal Forming

He, Dong, Ph.D. (China) 2009-09 to 2010-09, Harbin Institute of Technology, Harbin, P. R. China, China Scholarship Council

Kobayashi, Saturo, Prof. (Japan) 2010-06 to 2010-07, Tohoku University, Japan, Funded by Tohoku University, Japan

Kords, Cristoph, Dipl.-Ing. (Germany); 2009-02 to 2010-08, Ruhr-Universität Bochum, Funded by The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

Lebensohn, Riccardo, Prof. (Argentina/USA); 2010-02 to -2011-01, Los Alamos National Laboratory, USA, Humboldt Research Awardee

Maniruzzaman, Mohammad, Prof. (Bangladesh) 2009-02 to 2010-07, Islamic University, Kushtia, Bangladesh, Georg Forster Research Fellowship, Alexander von Humboldt Stiftung

Millán, Julio, M.Sc. (Venezuela), 2008-04 to 2011-09, Universidad Simón Bolívar, Venezuela, Fundayacucho-Caraca and German Academic Exchange Service (DAAD)

Pinto de Siqueira, Rodrigo, M.Sc. (Brasil) 2010-08 to 2010-10, University of Lorena, Brasil, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior

Salmi, Grégoire , M.Sc. (Spain); 2009-02 to 2009-04, Universidad Carlos III de Madrid, Spain, Funded by Universidad Carlos III de Madrid, Spain

Sandim, Hugo, Prof. (Brasil) 2009-09 to 2010-10, University of Lorena, Brasil, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior

Sato, Hisashi, Ph.D. (Japan); 2009-07, Nagoya Institute of Technology, Japan, Funded by Nagoya Institute of Technology, Japan

Svirina, Julia, Ph.D. (Russia) 2008-10 to 2008-12, Nizhny Novgorod State University, Russia, German Academic Exchange Service (DAAD) Scholarship

Tasan, Cem, Ph.D. (The Netherlands/Turkey) 2010-03 to 2012-02, Funded by M2i, Delft, The Netherlands

Verbeken, Kim, Dr. (Belgium) 2007-10 to 2012-09, Ghent University, Belgium, Research Foundation Flanders, Belgium

Voronova, Olena (Russia) 2009-04 to 2010-03, Funded by Otto Benecke Stiftung

Winning, Mirjam, PD Dr. (Germany) 2006-12 to – 2010-12, RWTH Aachen, Heisenberg Scholarship, German Research Foundation (DFG)

Zheng, Chengwu, Ph.D. (China) 2010-03 to 2011-06, Chinese Academy of Sciences, Shenyang, Liaoning, China, Alexander-von-Humboldt-Stiftung

Scientific Honours

2008 (not included in Scientific Report 2007/2008)

C. Zambaldi was awarded the IMPRESS Prize for Young Researchers by the European Space Agency in recognition of the uniqueness of the material science and application research within the IMPRESS project, 2008.

2009

Dr. rer. nat. A. A. Auer was appointed honorary professor at the TU Chemnitz, 2010-03.

A. Bobrowski obtained the first prize in the photo exposition on general metallography during the Metallographietagung in Aachen, 2009-09.

Dr.-Ing. U. Brüx and the Max-Planck-Institut für Eisenforschung received the first prize in the frame „Stahlinnovationspreis", category "Steel in Research and Development" for the development of TRIPLEX Steels, 2009-06.

Dr. rer. nat. M. Eumann, Prof. Dr. rer. nat. G. Sauthoff and Dr. rer. nat. M. Palm received the APDIC Best Paper Award of the Alloy Phase Diagram International Commission for the best published manuscript on alloy phase diagram data in the year 2008, 2009-05.

Dr. rer. nat. B. Grabowski was invited to the DFG-Nachwuchsakademie "Moderne Probleme der Materialwissenschaft und Werkstofftechnik", 2009-03.

Dr. rer.nat. A. W. Hassel was appointed professor for Chemical Technology of Inorganic Materials at the Johannes-Kepler-Universität Linz, Austria, 2009-07.

The Max-Planck-Institut für Eisenforschung GmbH has been honoured by the Chamber of Industry and Commerce (IHK) for its outstanding achievements in the training of apprentices, 2009.

Prof. Dr. P. Neumann was appointed honorary member of the „Deutsche Gesellschaft für Materialkunde (DGM)", 2009-06.

Prof. Dr.-Ing. D. Raabe has become Member of the German Council of Science and Humanities (German Wissenschaftsrat), 2009.

Prof. Dr.-Ing. D. Raabe has become Member of the Expert Committee in Materials Science and Engineering (MatSEEC) of the European Science Foundation, 2009-07.

M. Richter was awarded for his very good results in his final exams of the Chamber of Industry and Commerce (IHK) in the qualified job „Chemielaborant", 2009-05.

2010

Dr. rer. nat Y. Chen won the Chinese Government Award for Outstanding Self-Financed Student Abroad, Berlin, 2010-06.

Dr. rer. nat. C. Freysoldt received the Ψ_k Volker Heine Young Investigator Award for excellence of research involving electronic structure calculations, 2010-09.

Dr.-Ing. C. Herrera, Prof. Dr.-Ing. A. Padilha, and Prof. Dr.-Ing. R. L. Plaut have received the Best Poster Award for their contribution "Microstructure evolution during annealing treatment of austenitic stainless steels" on the 4th International Conference on Recrystallization and Grain Growth, 2010-07.

C. Kords has received the Springorum-Denkmünze of RWTH Aachen, 2010-06.

Dr. techn. K.J.J. Mayrhofer received the Hans-Jürgen Engell Prize, Nice, France, 2010-09.

F. Ram has received the 1st poster prize of the "Nucleation, Microstructure Evolution and Phase Transition" Symposium, MSE 2010, Darmstadt, Germany, 2010-08.

Dr.-Ing. S. Sandlöbes has received the "11th Willy-Korf-Award for Young Excellence" at the Steel Success Strategies XXV, New York, USA, 2010-06.

Dr.-Ing. S. Sandlöbes received the Friedrich-Wilhelm-Preis of the RWTH Aachen for outstanding scientific results presented in her thesis, 2010-10.

Dr. H.Sato, Dr.-Ing. S. Zaefferer and Prof. Dr. Y. Watanabe have received the 2010 Sawamura Award for their publication "In-situ observation of butterfly-type martensite in Fe-30mass%Ni alloy during tensile test using high-resolution EBSD", ISIJ International, Vol. 49 (2009), No.11, pp. 1784-1791, 2010.

Dr. rer. nat. Markus Valtiner received the Otto Hahn Medal of the Max Planck Society for his work on the „Atomistic Understanding of Structure, Stability and Adhesion at ZnO / Electrolyte Interfaces", 2010-06.

Dr. rer. nat. Markus Valtiner reiceived the Marie Curie International Outgoing Fellowship, 2010-02.

Dr. K. Verbeken received an honourable citation for the work "Methodologische optimalisatie van de elektrochemische technieken voor de studie van waterstofdiffusie in staal" van Dieter Simpelaere, Arcelor-Mittal award, Ghent University, 2010.

Participation in Research Programmes

National:

AICES (Aachen Institute for Advanced Study of Computational Engineernig Science)

EU-Regional School Trimester 2008/III "Materials Science"

BMBF (Federal Ministry of Education and Research)

Characterisation of final parts based on integral materials simulation along the process chain

Development of high performance materials for high-temperature heat exchanger and car-exhaust systems

Forging simulation AFP-steels

High resolution EPR spectroscopy of thin silicon films for solar energy science

Increase of competence in electrochemistry for electromobility – Kompetenzverbund Nord

Virtual development of ceramics and composite materials with tailored transport properties

BMWi (Federal Ministry of Economics and Technology)

Hydrogen induced embrittlement of cold rolls

Development of a novel wear-resistant material for industrial brake discs

BGR (Federal Institute for Geosciences and Natural Resources)

Metal corrosion in contact with clay

DAAD (German Academic Exchange Service)

Acciones integradas Hispano-Alemanas

DFG (German Research Foundation)

Ab initio description of temperature dependent effects in dimensionally constrained magnetic shape memory Heusler alloys

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

Accurate calculation of the electronic structure at grain boundaries via density functional theory and quasi particle corrections

Al-rich AlTi-alloys: Transformation of h-Al_2Ti and Al_5Ti_3 and formation of lamellar γ-TiAl + r-Al_2Ti microstructures

Antireflecting interlayers to increase transmission through thin metal films in spectroelectrochemical experiments

Atomic scale investigation of the kinetics of nano-precipitation in Fe-Si-Cu alloys using Atom Probe Tomography

Collaborative research centre 761: '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'

Collaborative research centre 761: 'Steel - ab initio. Quantum-mechanically guided design of new Fe-based alloys', partial project: Microstructure mechanics and the fundamentals of twinning'

Collaborative research centre 761: 'Steel - ab initio. Quantum-mechanically guided design of new Fe –based alloys', partial project: 'Defects and residual stresses in Fe-Mn-C steels'

Collaborative research centre 761: 'Steel - ab initio. Quantum-mechanically guided design of new Fe –based alloys', partial project: 'Atomic analysis of chemical gradients at interfaces by atom probe tomography '

Crustacean skeletal elements: variations in the constructional morphology at different hierarchical levels

Development and validation of a scale bridging description of heterogeneous deformation and intercrystalline failure of Molybdenum

Development of alternative, screening based, local Coupled Cluster methods and efficient algorithms for parallel architectures

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

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.

Highly accurate calculation of NMR schemical shift – method development, benchmarks and applications

High resolution scanning electron back scatter diffraction experiments of local crystallographic orientation patterning during plastic deformation

Interference and constrains of the impurity level of titanium alloys for recycling purposes

Investigation and characterization of the intermetallic phase formation of dissimilar Fe-Al joints produced by fast laser-based joining processes with large temperature gradients

Local mechanical properties of Mn-based steels

Materials world network: Physically based approach for predicting and minimizing damage nucleation in metals

Mechanical properties and interfaces of ultrafine grained materials by using 3D microscopy

Mechanisms of self and impurity diffuision in Fe-Al intermetallic compounds

Microstructure mechanics and fundamentals of twinning

Multiscale growth and doping simulations of nanostructured devices

Nanofluid mechanics

Non-equilibrium flow at gradient surfaces: Separation phenomena of multi-component fluids.

Non-equilibrium flow at gradient surfaces: Droplet kinetics and particle motion

Oxidation and segregation on high strength steels

Production of nanowire arrays through directional solidificaton and their application

Relationship between microstructure and damage mechanisms in multiphase steels

Research group 797 'Analysis and computation of microstructure in finite plasticity', partial project: 'Experimental analysis of the orientation dependence of deformation laminates'

Research priority program SPP 1204: Algorithms for the fast materials-oriented simulation of process chains in forming technology

Research Priority Program SPP 1296 'Heterogene Keim- und Mikrostrukturbildung: Schritte zu einem system- und skalenuebergreifenden Verstaendnis' – Partial Project: 'Elastic effects on heterogeneous nucleation and microstructure formation'

Scale-bridging studies of the elastic contributions to nucleation and initial microstructure formation in the eutectic system Ti-Fe

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

Helmholtz Society

Virtual institute for improving performance and productivity of integral structures through fundamental understanding of metallurgical reactions in metallic joints (VI-IPSUS)

Max Planck Society

Active coatings for corrosion protection

Characterisation of iron oxide nanoparticles

Computational mechanics of polycrystals

The nature of Laves phases

Triple-M: Max Planck Initiative on Multiscale Materials Modeling of Condensed Matter

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

State of North Rhine-Westphalia

Center for Electrochemical Sciences

Wilhelm und Else Heraeus-Stiftung e.V.

468. WE-Heraeus-Seminar: Ab initio Description of Iron and Steels

International:

Christian Doppler Society

Adhesion, electronic structure and mechanics of thin amorphous films on reactive metals

Analysis of the growth of thin amorphous films on zinc coated steel

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

Predictability of barrier and mechanical properties of organic/inorganic nanocomposite and multilayer films

Water at polymer/metal interfaces

European Union

Intermetallic materials processing in relation to earth and space solidification

Nextgenbiowaste 'Innovative demonstrations for the next generation of biomass and waste combustion plants for energy recovery and renewable electricity production'

Novel concepts for molecular interface engineering and unravelling of structure/proprty relationships at electrified interfaces

Surface engineered InGaN heterostructures on N-polar GaN-substrates for green light emitters

Foundation Materials Innovation Institute

Mobility of water and charge carries 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)

Advanced characterisation techniques for novel zinc-based alloy coating (ADCTEC)

High emissivity annealing technique (HEAT)

Hydrogen sensitivity of different advanced high strength microstructures (HYDRAMICROS)

Methodology of hydrogen measurement in coated steels (HPPM)

New approaches to quantitative hydrogen analysis of coated steel products (COATHYDRO)

Novel annealing procedures for improving HDG of HSS (NOVANNEAL)

Steady reactivity in hot-dip coating by direct deposit of iron oxides (Ferrigal)

Ultra-high strength and ductile FeMnAlC light-weight steels

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

Conferences, Symposia and Meetings Organized by the Institute

2009

M. Palm organized and chaired the 17th meeting of the Fachausschuss Intermetallische Phasen (technical committee "intermetallic phases") of the DGM at the MPIE on 2009-01-14.

R. Loschen organized the evaluation of IMPRS-SurMat. The meeting was held at the MPIE, 2009-04-23.

J. Neugebauer co-organized the CECAM-Workshop "Which Electronic Structure Method for the Study of Defects?", held at Lausanne/CH, 2009-06-08 to 2009-06-10.

J. Neugebauer co-organized the symposium "D31: Ab initio based modeling - designing new materials with electronic structure calculations" at the Euromat 2009 International Conference, held at Glasgow/GBR, 2009-09-07 to 2009-09-10.

P. Choi organized the Opening Ceremony for the new Atom Probe Tomography Laboratory and Scientific Symposium with 150 international participants, 2009-09-17.

F. Stein organized and chaired the Workshop "The Nature of Laves Phases XIII", which took place at the MPIE on 2009-11-11.

J. Neugebauer organized the Scientific Colloquium in honour of Peter Neumann, Düsseldorf, 2009-11-16.

T. Hickel co-organized the 448. Wilhelm und Else Heraeus-Seminar `Excitement in magnetism: Spin-dependent scattering and coupling of excitations in ferromagnets´, Ringberg, 2009-11-22 to 2009-11-25.

J. Neugebauer co-organized the symposium "LL: Mulitphysics Modeling in Materials Design" at the MRS Fall Meeting, Boston/USA, 2009-11-30 to 2009-12-04.

T. Hickel and J.Neugebauer organized the workshop "Ab initio Description of Iron, Steels and related materials", Düsseldorf 2009-12-16.

2010

M. Palm organized and chaired the 18th meeting of the Fachausschuss Intermetallische Phasen (technical committee "intermetallic phases") of the DGM at the GKSS-Forschungszentrum Geesthacht on 2010-01-13.

J. v. Pezold and J. Neugebauer organized the workshop "Computational Materials Science on Complex Energy Landscapes", Imst/Austria 2010-01-25 to 2010-01-29.

R. Loschen, L. Kienow and C. Tamura jointly with the Max Planck Foundation organized the "Unternehmergespräch der Max Planck Förderstiftung" at the MPIE, 2010-02-09.

A. Auer organized the "First Minisymposium on Perspectives in Quantum Chemistry for Electrochemistry" at RUB, Bochum, 2010-02-11.

J. Neugebauer organized the topical session (BV MatWerk) "Designing innovative structural materials and steels based on computational and experimental simulations" at the DPG Spring Meeting 2010, Regensburg, 2010-03-21 to 2010-03-26.

M. Stratmann, D. Raabe, J. Neugebauer and L. Kienow organized the Symposium on "Advanced Metallurgy and Combinatorial Synthesis of Metallic Materials" at the MPIE, 2010-06-22.

P.U. Biedermann organized and chaired the Polymer Day in the Series ICAMS Advanced Discussions, at the MPIE, 2010-06-23.

M. Palm, F. Stein and C. Tamura organized the commemorative colloquium in memory of Prof. Dr.-Ing. Georg Frommeyer at the Stahlinstitut VDEh, 2010-06-25.

F. Roters organized The Meeting of the Fachausschuss Computersimulation of the DGM in Cooperation with SFB 761 "steel ab initio" entitled „Werkstoffe ab initio -- Moderne Simulationsmethoden in der Werkstoffentwicklung" held at RWTH Aachen. 12 lectures were presented to about 25 participants from several countries, 2010-06-25.

B. Grabowski and J. Neugebauer co-organized the CECAM summer school on `Computational Materials Sciences´, San Sebastian/España, 2010-06-28 to 2010-07-03.

M. Valtiner co-organized and chaired the "Gordon Research Seminar on Aqueous Corrosion", New London, USA, from 2010-07-24 to 2010-07-25.

A. Auer organized the Second Minisymposium on "Challenges for Theory in Electrochemistry" at the MPIE, 2010-08-05.

R. Loschen and C. Tamura jointly with the Stahl-Zentrum organized the Tag der offenen Tür (Open Day) at the MPIE, Stahl-Zentrum and BFI, 2010-09-04.

J. Neugebauer co-organized the symposium "Crystalline, Amorphous, and Glassy Alloys" at the PSI-K Conference 2010, Berlin, 2010-09-12 to 2010-09-16.

T. Hickel, J. v. Pezold, J. Neugebauer and R. Drautz (ICAMS) organized the 468. Wilhelm und Else Heraeus-Seminar "Ab initio Description on Iron and Steels: Mechanical properties" at Ringberg castle, 2010-10-24 to 2010-10-29.

M. Palm co-organized and chaired the Symposium "Intermetallic-Based Alloys for Structural and Functional Applications" at the MRS Fall Meeting, Boston, USA from 2010-11-29 to 2010-12-02.

Institute Colloquia and Invited Seminar Lectures

2009

J. Schroers, Yale University, New Haven, CT, USA: Bulk Metallic Glass Forms like Plastics (2009-01-14, Colloquium)

F. H. Dalla Torre, ETH Zurich, Switzerland: Synthesis and Deformation Behaviour of Metallic Alloys with Different Internal Length Scales (2009-02-02, Colloquium)

A. Mortensen, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland : Replication Processing of Open-Pore Microcellular Aluminium (2009-02-12, Colloquium)

M. Wuttig, RWTH Aachen: Phase Change Alloys: A Challenge for Our Understanding of Amorphous and Crystalline Materials (2009-02-27, Colloquium)

W. G. Schmidt, Universität Paderborn: Optical Absorption of Water: Structural Effects and Many-Body Physics (2009-02-24)

A. Balducci, S. Passerini, University of Münster: Ionic Liquids as Electrolytes in Lithium Batteries (2009-03-03)

F. Liot, Linköping University, Sweden: Thermal Expansion of Ferromagnetic Fe-Based Alloys (2009-03-05)

T. Nishimura, University of Tokyo, Japan: Development of Oriented Inorganic/Organic Hybrid Materials Based on Biomineralization (2009-03-06)

H. S. Valberg, Norwegian University of Science and Technology (NTNU), Trondheim, Norway: Use of Advanced Internal Grid Patterns in Metals to Characterise Friction along Die Surfaces and Localised Heavy Deformations (2009-03-11)

E. Calvo, INQUIMAE, Buenos Aires, Argentina: Electron, Ion and Solvent Exchange in Redox Polyelectrolyte Self-Assembled Multilayers (2009-03-16)

M. J. Buehler, Massachusetts Institute of Technology, Cambridge, MA, USA: Deformation and Failure of Biological Protein Materials (2009-03-26)

J. K. Krüger, University of Luxembourg: The Generalized Cauchy Relation in Equilibrium and Non-Equilibrium of Oligomers, Polymers and Polymer Nanocomposites (2009-04-30)

A. Diaz Ortiz, Max Planck Institute for Metals Research, Stuttgart: Materials Cartography in Fe-Co Nanoscale Alloys (2009-05-04)

P. Bertoncello, Swansea University, U.K.: Functional Nanostructured Materials for Catalysis and Biosensing (2009-05-04)

G. Wilde, University of Münster: Interface-controlled Phase Equilibria in Nanocrystalline Materials (2009-05-05, Colloquium)

M. Arenz, Technische Universität München: Electrocatalytic Energy Conversion in PEM Fuel Cells (2009-05-11)

Z.-K. Liu, Penn State University, USA: Calculation of Magnetic Properties through Quantum, Statistics, and Modeling (2009-05-14, Colloquium)

A. Schneider, Benteler Stahl/Rohr GmbH, Paderborn: How to Make Steel Tubes Last Longer (2009-06-03, Colloquium)

M. Bouhassoune, University of Paderborn and Forschungszentrum Jülich (Helmholtz-Gesellschaft): Ab-initio Structural and Electronic Properties of Strained Silicon and High-k Materials based MOSFETS (2009-06-16)

A. Wixforth, University of Augsburg: Nano Quakes on a Chip: Surface Acoustic Waves for the Nanosciences (2009-06-23)

A. Aghajani, Ruhr-Universität Bochum: Microstructural Evolution in Creep-Resistant Steel (2009-06-25)

G. Dehm, Montanuniversität Leoben, Leoben, Austria: Small Scale Mechanical Testing: Challenges and Benefits (2009-06-29, Colloquium)

B. Hutchinson, Corrosion and Metals Research Institute (SWEREA-KIMAB), Stockholm, Sweden: The Great Goss Texture Mystery (2009-07-06)

J. Hirsch, Hydro Aluminium Deutschland GmbH, Research and Development, Bonn: Industrial Application of Simulation Tools Through Process Modelling in Aluminium Semi Production (2009-07-07, Colloquium)

A. Thiess (Forschungszentrum Jülich): Massively parallel KKR Green function method for large scale applications (2009-07-08)

A. Glensk, FH München: DFT description of rhenium clusters (2009-07-09)

H. Ehrlich, Max Bergmann Center of Biomaterials, Dresden University of Technology: Insights in Demineralization: Findings of Novel Biocomposites (2009-07-14)

Q. Feng: Study of single impurity Anderson model and dynamical mean field theory based on equation-of-motion method (2009-07-14)

S. Kobayashi, Tohoku University, Sendai, Japan: Characterisation of Microstructures in Multi-Component Alloys Using Bulk Combinatorial Method (2009-07-20)

D. Abu-Ras, Helmholtz Center Berlin for Materials and Energy, Berlin: Various electron microscopy techniques for analyses of thin-film solar cells (2009-07-28)

A. Abbasi, Technische Universität Chemnitz: Influence of dispersion interactions on the adsorption of organic semiconductors on coinage metal surfaces (2009-08-04)

J. Keckes, University of Leoben, Austria: In-Situ X-ray Diffraction as a Tool to Probe Mechanical Phenomena in Nano-structured Materials (2009-08-11)

M. Behr, RWTH Aachen: Modeling and Simulation in Computational Hemo- and Hydrodynamics, and Materials Processing (2009-08-14)

S. Pathak, EMPA - Swiss Federal Laboratories for Materials Testing and Research, Thun, Switzerland, Drexel University,Philadelphia, USA: Measurement of the Local Mechanical Properties in Polycrystalline Samples Using Spherical Nano-Indentation and Orientation Imaging Microscopy (2009-08-14)

R. Schmid-Fetzer, TU Clausthal: Computational Thermodynamics and Reactive Diffusion: Applications in Materials Science and Engineering (2009-08-18, Colloquium)

A. Gross, Universität Ulm: First-principles treatment of hydrogen adsorption and absorption at metal-vacuum and metal-water interfaces (2009-08-26)

D. Sander, Max-Planck-Institut für Mikrostrukturphysik, Halle: Stress beyond elasticity limits on surfaces and in atomic layers (2009-08-27)

M. Demura, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan: Texture memory effect in heavily cold-rolled Ni_3Al single crystals (2009-08-31)

K. Miyata, Sumitomo Metals, Japan: Current research activities in Sumitomo Metals - Microstructure and properties of ultra-fine grained steels by super short interval multi-pass rolling process - Effect of hydrogen on dislocation behavior in Ni-base super alloys (2009-09-01)

R. B. Wehrspon, Fraunhofer-Institut für Werkstoffmechanik, Halle: Clusters in Photovoltaics (2009-09-01, Colloquium)

R. Spatschek, ICAMS Ruhr-Universität Bochum: Structure Formation at Interfaces and Surfaces (2009-09-04)

D. Chrobak, University of Silesia, Katowice, Poland: Non-dislocation origin of the incipient plasticity in GaAs (2009-09-15)

J.H. Schneibel, Otto-von-Guericke-Universität Magdeburg: Ultrafine-grained Nanocluster Alloys with Extreme Creep Strength (2009-09-15, Colloquium)

M. Sugiyama, Nippon Steel Corporation, Japan: Recent progress in steel research of Nippon Steel (2009-09-16)

B. L. Adams, Brigham Young University, Provo, Utah, USA: EBSD-based microstructure characterization: from homogenization to localization (2009-09-21)

M. Strauss, Max Planck Institute of Biophysics: Biological Electron Microscopy: A Physicists Balancing Act (2009-09-11)

M. Takeyama, Tokyo Institute of Technology, Japan: Novel Design Concept for Advanced Austenitic Heat Resistant Steels Strengthened by Laves Phase (2009-09-28, Colloquium)

K. Parlinski, Polish Academy of Sciences: Ab initio Phonon Calculations in Crystals (2009-09-29, Colloquium))

S. Wessel, Institut für Theoretische Physik III, Universität Stuttgart: Monte Carlo Methods for Quantum Spin Systems (2009-10-13)

P. Schaaf, Ilmenau University of Technology: The Iron-Nitrogen and Iron-Carbon-System and Cast Iron: "Old" Systems Forever Young (2009-11-02, Colloquium)

A. Bagrets, Institut für Nanotechnologie, Forschungszentrum Karlsruhe: Electron transport through atomic wires and molecular junctions: density functional theory description (2009-11-05)

N. Sandschneider, Humboldt Universität zu Berlin: Current-induced Switching of Magnetization (2009-11-10)

M. Wagner, Ruhr-Universität Bochum: On Challenges in Processing and a New Understanding of the Mechanical Properties of NiTi Shape Memory Alloys (2009-11-09, Colloquium)

W. Schmickler, University of Ulm: Theory of Hydrogen Evolution on Metal Surfaces and Nanostructures (2009-11-10, Colloquium)

M. Umemoto, Toyohashi University of Technology, Japan: Strengthening and Grain Refinement in Steels by Severe Plastic Deformation (2009-11-25)

T. Woodcock, IFW Dresden: Multi-Phase Local Texture Analysis in NdFeB Sintered Magnets (2009-11-30)

P. Grammatikopoulos, University of Liverpool: Computer Simulation of Dislocation Interaction with Radiation-induced Obstacles in Iron (2009-12-09)

R. Janisch, ICAMS Ruhr-Universität Bochum: Micromechanical modelling of macroscopic material behaviour: Mechanical properties of interfaces – insights from atomistic simulations (2009-12-10)

Y. N. Gornostyrev, Institute on Quantum Materials Science (IQMS), Ekaterinburg, Russia: research activities at the IQMS (2009-12-16)

A. I. Lichtenstein, University Hamburg: research activities on correlated electron systems at Hamburg University (2009-12-16)

V. Kokotin, Topological criteria for the glass forming ability (2009-12-21)

2010

Ch. Wöll, Institut für Funktionelle Grenzflächen (IFG), Karlsruher Institut für Technologie (KIT), Eggenstein-Leopoldshafen: Interfacial Systems Chemistry: Highly Ordered Systems as Basis for Hierarchical Architectures (2010-01-15)

S. Roke, Max Planck Institute for Metals Research, Stuttgart: Viewing the molecular structure of nanoscopic droplets and particles (2010-01-15)

C. E. Nebel, Fraunhofer-Institute of Applied Solid State Physics, Freiburg: From nano- to single-crystalline diamond: properties and applications (2010-01-18)

A. Fischer, Universität Duisburg-Essen: Sliding Wear – Severe Plastic Deformation, Mechanical Mixing and Fatigue (2010-01-19)

A. Glensk, EPFL Lausanne/CH: Integrated approach to develop thermodynamic and thermophysical key data for solidification of aluminium alloys (2010-01-19)

U. Gerstmann, Universität Paderborn: ab initio calculation of the electronic g-tensor of paramagnetic structure (2010-01-20)

M. Vsianska, University of Brno/CZ: Ab initio study of segregation of impurities at grain boundaries and surfaces in nickel (2010-01-21)

G. M. Pharr, University of Tennessee and Oak Ridge National Laboratory, Knoxville, Tennessee, USA: From Pop-in to Pillars: The Utility of Nanoindentation in Probing the Mechanisms of Plasticity at Small-Scales (2010-01-26)

W. Blum, University Erlangen-Nürnberg, Erlangen: Dislocation walls and strength of crystalline solids – is the composite model of plastic deformation valid? (2010-01-28)

M. Tagliazucchi, University of Buenos Aires, Argentine: Electrodes modified with self-assembled polyelectrolyte multilayers (2010-02-04)

E. P. Elsukov, Physical-Technical Institute, Izhevsk, Russia: Nanostructure and phase formation under severe mechanical treatment of Fe-based systems (2010-02-10)

A. Prößdorf, Paul-Drude-Institut Berlin: Self-assembled GaSb nano islands on Si 111 surfaces (2010-02-11)

P. Littlewood, Oxford University, UK: Deformation of Ti-6-4 at the microstructural scale (2010-02-23)

R. Lebensohn, Los Alamos National Laboratory, Los Alamos, NM, USA: Crystal Plasticity Fast Fourier Transform-based formulation: theory, implementation and examples (2010-02-24)

G. He, Universität Düsseldorf: Shear-induced stretching of polymer chains (2010-02-24)

P. R. Rios, Universidade Federal Fluminense (UFF), Brazil: Application of average N-hedra (ANHs) for the description of polyhedral grains (2010-02-26)

M. Moseler, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg: Atomistic Insights into the Tribological Properties of Diamond and Diamond-Like Carbon (2010-03-03)

C. Race, Imperial College London/U.K.: Adding quantum mechanical electrons to atomistic simulations of radiation damage in metals (2010-03-10)

D. Holec, University of Leoben, Austria: Phase stability of pseudo-binary nitride alloys (2010-03-17)

D. Camaco: Structural, electronic and optical properties of GaN/AlN semiconductor heterostructures (2010-03-30)

R. Würz, Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Stuttgart: Cu(In,Ga)Se2 thin-film solar cells on flexible steel substrates (2010-03-31)

W. A. Kopp, RWTH Aachen: Ab Initio Calculation of Elementary Reactions for the Combustion Process Development (2010-03-31)

G. Kresse, University of Vienna, Austria: The Random Phase Approximation to the Correlation Energy: Solids and Surfaces (2010-04-13, Colloquium)

S. Okatov, CJSC Institute Ekaterinburg, Russia: Ab initio calculations of non-ideal iron (2010-04-14)

M. Himmerlich, Technische Universität Ilmenau: Surface electronic properties and molecule interaction of clean group III-nitride and nanocrystalline indium oxide thin films (2010-05-06)

R. Magerle, TU Chemnitz: Imaging Structure Formation Processes in Nanostructured Polymeric Fluids (2010-05-11, Colloquium)

H. Sharma, Delft University of Technology, The Netherlands: 3-dimensional analysis of microstructures (2010-05-12)

A. Schindlmayr, Universität Paderborn: Spin excitations in itinerant ferromagnets from first principles (2010-05-18)

R. Marceau, The University of Sydney, Australia: Outlook for Design in 2xxx Al Alloys (2010-06-02)

C. Cáceres, University of Queensland, Brisbane, Australia: Grain Size Hardening in Mg and Mg-Zn Solid Solutions (2010-06-17)

A. Duff, Delft University of Technology, NL: Ab-initio and semi-empirical study of B, C and N behaviour in ferrite (2010-06-18)

K. Xie, University of Sydney, Australia: Ageing behaviour of Nb-microalloyed CASTRIP steels (2010-06-21)

A. Barnoush, Universität des Saarlandes, Saarbrücken: Local examination of hydrogen embrittlement in metals (2010-06-24)

S. C. Vogel, Los Alamos Neutron Science Center, Los Alamos, New Mexico, USA: The HIPPO Beam-line at LANSCE (2010-06-29)

Y. Politi, Max Planck Institute of Colloids and Interfaces, Potsdam-Golm, Germany: Magnesium Ion in Biomineralization: Understanding its role in stabilization of Amorphous Calcium Carbonate (2010-6-29)

C. M. Cady, Los Alamos National Laboratories, Los Alamos, New Mexico, USA: Characterization of a Uranium-Niobium Alloy Over a Range of Temperatures and Strain Rates (2010-07-01)

L. R. Bairi, Indira Gandhi Centre for Atomic Research, Kalpakkam, India: Corrosion Resistant Type 316SS-Zirconium Metal Waste Form Alloys for Geological Disposal (2010-07-05)

Ch. Van de Walle, University of California, Santa Barbara/USA: Controlling the Conductivity of Transparent Oxides (2010-07-05)

N. Plumere, Ruhr University Bochum/Center for Electrochemical Sciences: Supported Catalysis and Electrochemistry (2010-07-07)

M. Kibalchenko, Cambridge University, UK: Identification of electronic and structural properties through first principles NMR calculations (2010-07-09)

M. Watanabe, Lehigh University, Bethlehem, Pennsylvania, USA: Atomic-resolution chemical analysis and nano-order grain-orientation analysis in scanning transmission electron microscopy (2010-07-12)

K. Ushioda, Nippon Steel, Chiba, Japan: Control of recrystallization texture in steels (2010-07-13)

M. Biesheuvel, Wageningen UR, Wageningen, The Netherlands: Double layer effects in colloidal interactions and in electrochemistry: the Frumkin effect and porous electrodes (2010-07-19)

C. S. Hartley, El Arroyo Enterprises LLC, Sedona, Arizona, USA: The Dislocation Density Vector (DDV) and Discrete Dislocation Dynamics (DDD) Simulations (2010-07-27)

M. Sugiyama, Nippon Steel Corporation, Chiba, Japan: Electron Channeling Contrast Imaging of Dislocations in SEM and 3D Morphology of Martensite Island in Bainitic Steels (2010-08-26)

A. Rosenauer, Universität Bremen: Towards quantitative Scanning Transmission Electron Microscopy (STEM) in III-Nitride semiconductors (2010-09-08)

K. Mukherjee, RWTH Aachen: Grain refinement and modelling techniques in dual phase steels (2010-09-08)

P. Kölsch, Karlsruhe Institute of Technology: In situ characterization of biointerfaces using sum-frequency generation (SFG) spectroscopy (2010-09-20)

E. Rauch, SIMAP laboratory, Grenoble, France: Measuring misorientations and grain sizes in severely deformed metals through orientation mapping on a Transmission Electron Microscope (2010-09-24)

R. Zarnetta, Ruhr-Universität Bochum: Advanced Metallurgy and Combinatorial Synthesis of Metallic Materials (2010-09-24)

A. Bandarenka, Ruhr-Universität Bochum: Combining DFT-calculations and experimental electrochemistry: Examples of applications in electrocatalysis, Center for Electrochemical Sciences (2010-10-13)

F. La Mantia, Ruhr-Universität Bochum: A Critical Analysis on the Use of Mott-Schottky Plots to Characterise the Passive Film/Electrolyte Junction (2010-10-20)

E. Kozeschnik, Vienna University of Technology, Vienna, Austria: Modeling Precipitation in Crystalline Materials from the atomistic to the continuum scale (2010-10-21, Colloquium)

C. Elsässer, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg: First-Principles Modelling of Dopants at Interfaces in TCO Materials (2010-11-09, Colloquium)

J. LLorca, Madrid Institute for Advanced Studies of Materials (IMDEA Materials Institute) & Department of Materials Science, Polytechnic University of Madrid: Computational materials engineering – an application of multiscale modeling of materials (2010-11-23)

Lectures and Teaching at University

2009

A. Erbe, Ruhr-Universität Bochum: Spectroscopy at Interfaces (Lecture and Exercise), WS 2008/2009, WS 2009/2010.

T. Hickel, Ruhr-Universität Bochum: Moderne Computersimulations-Methoden in der Festkörperphysik, WS 2009/2010.

M. Palm, Charles University Prague, Czech Republic, School of Iron Aluminides: Ternary Fe-Al-X Systems, 2009-09-21.

D. Raabe, MPIE Düsseldorf, Lecture for International Max Planck Research School SurMat: Crystal and crystal plasticity, 2009-03-18 to 2009-03-19.

D. Raabe, RWTH Aachen: Micromechanics of Materials (Lecture 3 and Exercise 1), (Master classes in English language), SS 2009.

D. Raabe, RWTH Aachen: Die Geschichte der Werkstoffe (History of Metallurgy) in der RWTH Ringvorlesungsreihe Einführung in die Werkstofftechnik (Lecture 1 and Exercise 1), SS 2009.

F. U. Renner, A. W. Hassel, A. Erbe, P. Keil, D. Sanders, MPIE Düsseldorf, Lecture for International Max Planck Research School SurMat: Physical Chemistry of Surfaces and Interfaces, 2009-10-19 to 2009-10-30.

M. Rohwerder and M. Stratmann, Ruhr-Universität Bochum: Korrosion, SS 2009.

F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2008/2009, WS 2009/2010.

F. Stein, Charles University Prague, Czech Republic, School of Iron Aluminides: The Binary Fe-Al System, 2009-09-21.

K. Verbeken, Ghent University, Belgium: Course 'Materiaaltechnologie', responsible for teaching part of the practical classes, WS 2008/2009.

M. Winning, RWTH Aachen: Theoretische Metallkunde II (Lecture 2 and Exercise 1), SS 2009.

S. Zaefferer, FU Berlin: Short course on the fundamentals of texture and EBSD-based orientation microscopy, 2009-03-11 to 2009-03-13.

S. Zaefferer, MPIE Düsseldorf, Lecture for International Max Planck Research School SurMat: Analytical transmission and scanning electron microscopy, 2009-03-24 to 2009-03-25.

S. Zaefferer, MPIE Düsseldorf: Lecture series on scanning electron microscopy and electron backscatter diffraction, October 2009 – December 2009.

2010

A. A. Auer, TU Chemnitz: Grundlagen von Elektronenstrukturrechnungen, SS 2010.

A. Erbe, Ruhr-Universität Bochum: Spectroscopy at Interfaces (Lecture and Exercise), WS 2010/2011.

T. Hickel, J. Neugebauer, Ruhr-Universität Bochum: Computerpraktikum - Moderne Computersimulations-Methoden in der Festkörperphysik, SS 2010.

T. Hickel, J. Neugebauer, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2010/2011.

J. Neugebauer, Ruhr-Universität Bochum, ICAMS, Lecture for International Max Planck Research School SurMat: Fundamentals of ab initio simulations and their application to surface physics, 2010-02-22.

D. Raabe, RWTH Aachen: Micromechanics of Materials (Lecture 3 and Exercise 1), (Master classes in English language), SS 2010.

D. Raabe, RWTH Aachen: Die Geschichte der Werkstoffe (History of Metallurgy) in der RWTH Ringvorlesungsreihe Einführung in die Werkstofftechnik (Lecture 1 and Exercise 1) SS 2010.

M. Rohwerder and M. Stratmann, Ruhr-Universität Bochum: Korrosion, SS 2010.

F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, SS 2010.

K. Verbeken, Ghent University, Belgium: Co-lecturer for the bachelor course 'Milieutechnologie' (6SP), lecturer Prof. Thybaut (IR12) and Prof. Schoukens (IR11), 2010 – present.

K. Verbeken, Ghent University, Belgium: Responsible for course 'Corrosie en oppervlaktetechnologie' (4SP), co-lecturer Prof. Verhaege, 2010 – present.

K. Verbeken, Ghent University, Belgium: Co-lecturer for the course 'Duurzaamheid van materialen' (4SP), lecturer Prof. De Belie (IR14), 2007 – present.

K. Verbeken, Ghent University, Belgium: Replacing Prof. Verhaege for teaching the partim corrosion of the course 'Corrosie en oppervlaktetechnologie', 2007-2010.

K. Verbeken, IVPV – Ghent University, Belgium: Co-teaching 2 modules of 7 evening-classes each with Prof. Houbaert – 'Materialenkennis', 2010-2011.

M. Winning, RWTH Aachen: Theoretische Metallkunde II (Lecture 2 and Exercise1), SS 2010.

S. Zaefferer, RWTH Aachen: Microstructures, Microscopy and Modelling, International Masterclass on Materials Technology, SS 2010.

S. Zaefferer, T. Hickel, U. Prahl (RWTH), RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2010.

Invited Talks at Conferences and Colloquia

2008 (not included in Scientific Report 2007/2008)

Demir, E., Raabe, D. and Zaefferer, S.: *Quantification of Geometrically Necessary Dislocations Beneath Small Indents of Different Depths Using EBSD Tomography.* (MRS Fall Conference 2008, Boston, USA, 2008-12-01 to 2008-12-05).

Fabritius, H., Sachs, C., Nikolov, S., Romano, P., Hild S. and Raabe, D.: *Wie beeinflussen Struktur und chemische Zusammensetzung auf unterschiedlichen Längenskalen die mechanischen Eigenschaften von biologischen Materialien?* (Institute Colloquium, Department of Polymer Science, Johannes Kepler University Linz (JKU), Austria, 2008-11-20).

Fabritius, H., Sachs, C., Nikolov, S., Romano, P., Hild, S. and Raabe D.: *Influence of Structural Principles at Different Length Scales on the Mechanics and Functional Efficiency of Biological Materials.* (Ringberg Symposium 2008: Biological Approaches in Materials Sciences, Rottach-Egern, Germany, 2008-10-01 to 2008-10-04).

Ma, D., Raabe, D., Friák, M. and Neugebauer, J.: *Ab Initio Based Multiscale Alloy Design.* (Mater. Sc. Techn. Conference 2008; Symposium on Discovery and Optimization of Materials through Computational Design, Pittsburgh, USA, 2008-10-05 to 2008-10-09)

Mason, D. E., Bieler, T. R., Boehlert, C., Crimp, M. A., Wang, L., Yang, Y., Eisenlohr, P., Roters, F. and Raabe, D.: *Computational Modeling of Interactions Between Slip-Systems and Grain Boundaries that Lead to Fracture Initiation.* (4th International Conference on Multiscale Materials Modeling, Tallahassee, USA, 2008-10-27 to 2008-10-31).

Nikolov, S., Petrov, M., Friák, M., Raabe, D., Sachs, C., Fabritius, H., Neugebauer, J. and Lymperakis, L.: *Hierarchical Modeling of the Elastic Properties of Lobster Cuticle via Ab Initio Calculations and Mean-field Homogenization.* (MRS Fall Conference 2008, Boston, USA, 2008-12-01 to 2008-12-05).

Raabe, D., Roters, F., Counts, A., Friák, M. and Neugebauer, *J.: Polycrystal Mechanics.* (Physics Department, University Münster, Germany, 2008-11-13).

Todorova, M.: *Oxidation von Übergangsmetalloberflächen* (Universität Paderborn, Technische und Makromolekulare Chemie, Universität Paderborn, Germany, 2008-12-17).

von Pezold, J.: *Ab initio based approaches to failure mechanisms in steels: Application to hydrogen embrittlement.* (Materialphysikalisches Seminar Georg August Universität Göttingen, Göttingen, Germany, 2008-12-18).

2009

Bieler, T. R., Crimp, M. A., Yang, Y., Wang, L., Eisenlohr, P., Roters, F., Raabe, D., Liu, W., Ice, G. and Mason, D. E.: *Interactions Between Slip-Systems, Grain Boundaries, Heterogeneous Deformation, and Microcracking in Commercially Pure Ti.* (International Plasticity Conference 2009, Virgin Islands, USA, 2009-01-03 to 2009-01-08).

Counts, W.A., Friák, M., Raabe, D. and Neugebauer, J.: *Ab Initio Determined Materials-Design Limits in Ultra Light-Weight Mg-Li Alloys.* (8th International Conference on Magnesium Alloys and their Applications, Weimar, Germany, 2009-10-26 to 2009-10-29).

Dick, A.: *First Principles Predictions of Stacking Fault Properties in FeMn Alloys.* (Asia Steel 2009, Busan, Republic of Korea, 2009-05-24 to 2009-05-27).

Eisenlohr, P., Demir, E., Roters, F. and Raabe, D.: *A Non-Local Dislocation Based Constitutive Hardening Model in Crystal Plasticity Finite FEM.* (MRS Fall Meeting 2009, Boston, USA, 2009-11-30 to 2009-12-04).

Eisenlohr, P., Tjahjanto, D. D., Roters, F. and Raabe, D.: *Analysis of the Relaxed Grain Cluster Polycrystal Homogenization Scheme in Texture Prediction.* (ICSMA-15, 15th International Conference on the Strength of Materials, Dresden, Germany, 2009-08-16 to 2009-08-21).

Erbe, A. and R. Sigel*: Ellipsometric light scattering for probing the interface of colloidal particles.* (Advanced Polarimetric Instrumentation, Palaiseau, France, 2009-12 to 2009-12).

Fabritius, H., Nikolov, S., Sachs, C., Hild S., Raabe, D., Petrov, M., Lymperakis, L., Friák, M. and Neugebauer J.: *Arthropod Cuticle: a Biological Multifunctional Composite Used as Template for Ultiscale Modelling.* (NCTAM 2009, 11th National Congress on Theoretical and Applied Mechanics, Borovets, Bulgaria, 2009-09-02 to 2009-09-05).

Freysoldt, C.:*What can EPR hyperfine parameters tell about the Si dangling bond? A theoretical viewpoint.* (1st International Workshop on the Staebler-Wronski effect, Berlin, Germany, 2009-04-20 to 2010-04-23).

Freysoldt, C.: *Fully ab initio finite-size corrections for charged defects in the supercell approach.* (CECAM-Workshop, Lausanne, Switzerland, 2009-06-08 to 2009-06-10).

Friák, M.: *Ab initio density functional calculations.* (CCMX Summer School Course "Modelling in Materials Science: Theory and Applications", Lausanne, Switzerland, 2009-08-26 to 2009-08-28).

Friák, M., Counts, W.A., Raabe, D. and Neugebauer, J.: *Fundamental materials-design limits in ultra-light weight Mg-Li alloys identified via ab initio calculations*. (Max Planck Institute for Metals Research, Stuttgart, Germany, 2009-07-24).

Friák, M., Counts, W.A., Raabe, D. and Neugebauer, J.: *Ab initio determined materials-design limits in ultra light-weight Mg-Li alloys*. (Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 2009-07-21).

Friák, M., Deges, J., Krein, R., Stein, F., Palm, M., Frommeyer, G. and Neugebauer, J.: *Combining Experimental and Computational Methods in the Development of Fe$_3$Al-based Materials*. (5th Discussion Meeting on the Development of Innovative Iron Aluminium Alloys (FEAL 2009), Prague, Czech Republic, 2009-09-21 to 2009-09-24).

Friák, M., Kim, O., Sob, M., Ismer, L. and Neugebauer, J.: *Ab initio calculation of phase boundaries in iron along the bcc-fcc transformation path and magnetism of iron overlayers*. (Montan University Leoben, Austria, 200-07-09).

Friák, M., Nikolov, S., Petrov, M., Sachs, C., Fabritius, H.-O. and Ma, D.: *Ab-initio based multi-scale approaches to the elasticity of metallic polycrystals and hierarchical biocomposites*. (ICAMS Colloquium, Bochum, Germany, 2009-10-19).

Friák, M., Nikolov, S., Petrov, M., Sachs, C., Fabritius, H.-O., Ma, D., Lymperakis, L., Raabe, D. and Neugebauer, J.: *Multi-scale elastic properties of hierarchical biocomposites*. (Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 2009-10-13).

Friák, M., Nikolov, S., Petrov, M., Sachs, C., Ma, D., Fabritius, H., Lymperakis, L., Raabe, D. and Neugebauer, J.: *Ab-initio based multi-scale approaches to the elasticity of metallic polycrystals and hierarchical biocomposites*. (XI National Congress on Theoretical and Applied Mechanics, Borovets, Bulgaria, 2009-09-02 to 2009-09-05).

Friák, M., Sander, B., Ma, D., Counts, W.A., Raabe, D. and Neugebauer, J.: *Ab-initio based multi-scale approaches to the elasticity of polycrystals (Ti-based alloys for medical applications)*. (Montan University Leoben, Austria, 2009-07-08).

Friák, M., Zhu, L.-F., Dick, A., Hickel, T. and Neugebauer, J.: *First-principles study of the Ti-Fe eutectic system*. (Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 2009-09-24).

He, C., Stein, F. and Palm, M.: *Thermodynamic assessment of the Nb-Co and Nb-Co-Al system* (2nd Sino-German Symposium on Computational Thermodynamics and Kinetics and Their Applications to Solidification, Aachen/Kornelimünster, 2009-06-08 to 2009-06-12).

Hickel, T.: *Computational Phase Studies: Deriving free energies and phase transitions from first principles*. (MRS 2009 Fall Meeting, Boston, USA, 2009-11-30 to 2009-12-04).

Hickel, T.: *First principles determination of thermodynamic properties in metals*. (ICAMS Colloquium, Bochum, Germany, 2009-01-19).

Hickel, T., Grabowski, B., Körmann, F., Dick, A. and Neugebauer, J.: *The accuracy of first principles methods in predicting thermodynamic properties of metals*. (International Material Research Conference, Cancun, Mexico, 2009-08-16 to 2009-08-21).

Hickel, T., Grabowski, B., Körmann, F., Dick, A. and Neugebauer, J.: *The accuracy of first principles methods in predicting thermodynamic properties of metals*. (Asia Steel 2009, Busan, Republich of Korea, 2009-05-24 to 2009-05-27).

Hickel, T., Körmann, F., Dick, A. and Neugebauer, J.: *Considerations on the magnetic contribution to the free energy of Fe and related alloys* (MCA-Fe. International workshop "Modern computational approaches in iron based alloys, Ekaterinburg, Russian Federation, 2009-10-01 to 2009-10-03).

Hickel, T., Uijttewaal, M., Grabowski, B. and Neugebauer, J.: *First principles determination of phase transitions in magnetic shape memory alloys*. (2nd Sino-German Symposium on Computational Thermodynamics and Kinetics and their Application to Solidification, Aachen / Kornelimünster, Germany, 2009-06-08 to 2009-06-12).

Liu, T.: *Texture Formation Process, Related Macro-Stresses and Electrical Conductivity Mechanism of CVD Diamond Films' and 'Electrical Conductivity Mechanism of CVD Diamond Films*. (Agency of Science, Technology and Research (A*STAR), Singapore, 2009-08).

Ma, D., Friák, M., Knezevic, M., Kalidindi, S. R., Lebensohn, R., Roters, F., Neugebauer, J. and Raabe, D.: *Polycrystal Coarse Graining of Elastic Properties for Ti-Nb Biomedical Grades Using Ab-Initio Single Crystal Elastic Constants*. (International Plasticity Conference 2009, Virgin Islands, USA, , 2009-01-03 to 2009-01-08).

Neugebauer, J.: *Materials design based on ab initio thermodynamics: Development of accurate and efficient multiscale strategies* (Workshop IWOM-3, Berlin, Germany, 2009-03-10 to 2009-03-13).

Neugebauer, J.: *Understanding and designing engineering materials based on ab initio thermodynamics*. (Workshop PennState University, Pennsylvania, USA, 2009-03-19).

Neugebauer, J.: *Ab Initio Based Multiscale Modeling of Engineering Materials: From a Predictive Thermodynamic Description to Tailored Mechanical Properties* (Colloquium at TU Bergakademie Freiberg, Germany, 2009-05-06).

Neugebauer, J.: *Ab Initio Based Multiscale Modeling of Engineering Materials: From a Predictive Thermodynamic Description to Tailored Mechanical Properties.* (Asia Steel Conference, Busan, Republic Of Korea, 2009-05-24 to 2009-05-27).

Neugebauer, J.: *Challenge and opportunities for the European Steel Industry* (Asia Steel Conference, Busan, Republic Of Korea, 2009-05-24 to 2009-05-27).

Neugebauer, J.: *Multi-Scale Computational Materials Design of Structural Materials: First-Principles Calculations* (Workshop on Multi-Scale Computational Materials Design of Structural Materials, Republic of Korea, 2009-05-29).

Neugebauer, J.: *Materials Design Based On Ab Initio Thermodynamics And Kinetics: Present Status And Perspectives.* (Colloquium at Universität Gießen, Germany, 2009-06-05).

Neugebauer, J.: *Computing free energy contributions of point defects* (CECAM/PSI_K-Workshop, Lausanne, Switzerland, 2009-06-8 to 2009-06-11).

Neugebauer, J.: *Ab Initio Thermodynamics: Status, Applications and Challenges* (2nd Sino-German Symposium, Aachen, Germany, 2009-06-9 to 2009-06-12).

Neugebauer, J.: *Materials Design based on Ab Initio Thermodynamics: Status, Perspectives, and Applications.* (Colloquium at Universität Stuttgart, Germany, 2009-07-02).

Neugebauer, J.: *Material- und Werkstoffdesign am Computer: Möglichkeiten, Grenzen und Perspektiven.* (Akademie der Wissenschaften, Düsseldorf, Germany, 2009-09-11).

Neugebauer, J.: *Computing the free energy: Possibilities, challenges and limitations of present day ab initio techniques.* (Workshop Modern computational approaches in iron based alloys, Jekaterinburg, Russian Federation, 2009-10-1 to 2009-10-3).

Neugebauer, J.: *Chancen und Grenzen der ab initio-Modellierung* (Workshop Industrieberaterkreis SFB761, Aachen, Germany, 2009-10-14).

Nikolov, S., Sachs, C., Fabritius, H., Raabe, D., Petrov, M., Friák, M. and Neugebauer, J.: *Modeling of the Mechanical Properties of Lobster Cuticle from Ab Initio to Macroscale: How Nature Designs Multifunctional Composites with Optimal Properties.* (International Plasticity Conference 2009, Virgin Islands, USA, 2009-01-03 to 2009-01-08).

Ohsaki, S., Raabe, D. and Hono, K.: *Mechanical Alloying and Amorphization in Cu-Nb-Ag In Situ Composite Wires Studied by TEM and Atom Probe Tomography.* (MRS Fall Meeting, Boston, USA, 2009-11-30 to 2009-12-04)

Palm, M.: *Intermetallic phases for structural applications at high temperatures* (DPG Frühjahrstagung, Dresden, Germany, 2009-03-23 to 2009-03-27).

Palm, M.: *Recent progress in the development of Fe-Al-based materials.* (THERMEC' 2009 – International Conference on Processing & Manufacturing of Advanced Materials, Berlin, 2009-08-25 to 2009-08-29).

Ponge, D., Dmitrieva, O., Millán, J., Sander, B., Kostka, A. and Raabe, D.: *Ultra High Strength Steel Design by Using Nanoparticles.* (The 2nd International Symposium on Steel Science (ISSS 2009), Kyoto, Japan, 2009-10-21 to 2009-10-24).

Raabe, D., Roters, F., Demir, E., Weber, F., Ma, D., Zaafarani, N. and Zaefferer, S.: *3D Analysis of Size Dependent Crystal Plasticity by Using Tomographic EBSD and Crystal Plasticity FEM.* (International Plasticity Conference 2009, Virgin Islands, USA, 2009-01-3 to 2009-01-08)

Raabe, D.: *The Mechanics of Crystals.* (Academy of Science of North-Rhine-Westphalia, Düsseldorf, Germany, 2009-11-04).

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2010

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X. Wu: Characterization and comparison of structural coloration in the elytra of three *Carabus* ground beetle species. RWTH Aachen (2009).

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D. Hessling: Die Erstarrung in der Kugel: Die Methode der Sonometallurgie. Fachhochschule Düsseldorf (2010).
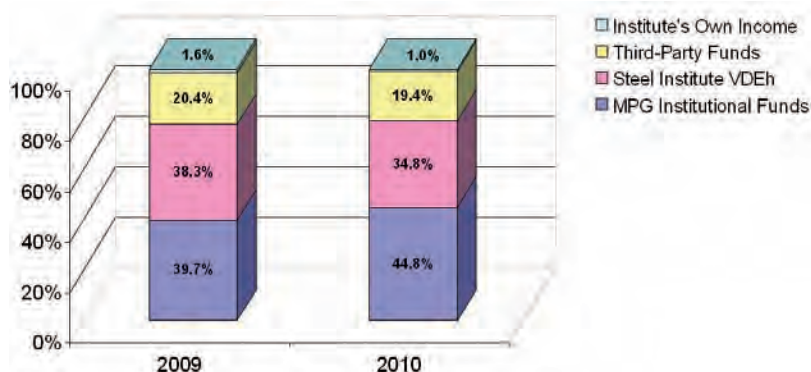
N. Tillack: Monte-Carlo-Simulationen zu Mn-Stählen mit Nano-Precipitates, Ruhr-Universität, Bochum (2010)
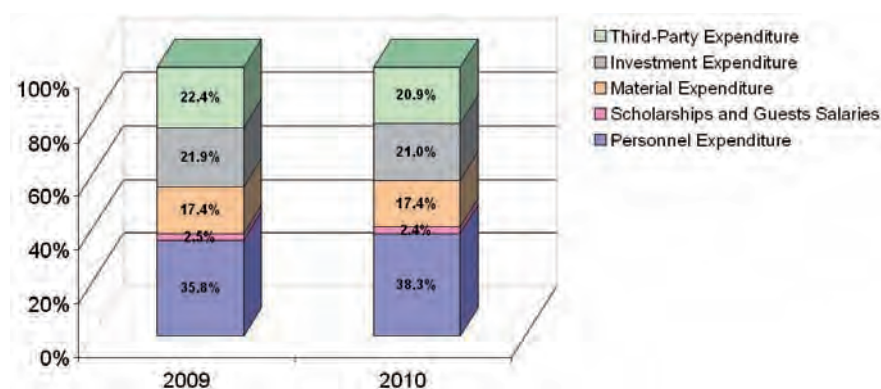
Budget of the Institute

Revenue
(percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2010 data estimated)

Legend:
- Institute's Own Income
- Third-Party Funds
- Steel Institute VDEh
- MPG Institutional Funds

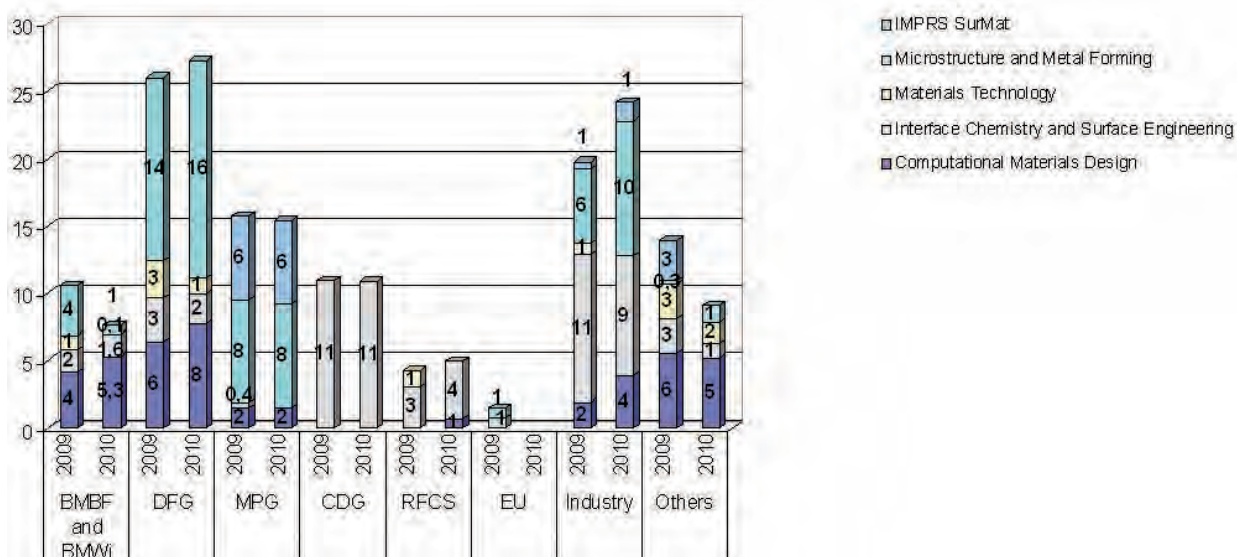|	2009	2010
Institute's Own Income	1.6%	1.0%
Third-Party Funds	20.4%	19.4%
Steel Institute VDEh	38.3%	34.8%
MPG Institutional Funds	39.7%	44.8%

Expenditure
(percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2010 data estimated)

Legend:
- Third-Party Expenditure
- Investment Expenditure
- Material Expenditure
- Scholarships and Guests Salaries
- Personnel Expenditure

	2009	2010
Third-Party Expenditure	22.4%	20.9%
Investment Expenditure	21.9%	21.0%
Material Expenditure	17.4%	17.4%
Scholarships and Guests Salaries	2.5%	2.4%
Personnel Expenditure	35.8%	38.3%

Third-Party Funds
(percentual contributions to total revenue including personnel, material, investments; year 2010 data estimated)

Legend:
- IMPRS SurMat
- Microstructure and Metal Forming
- Materials Technology
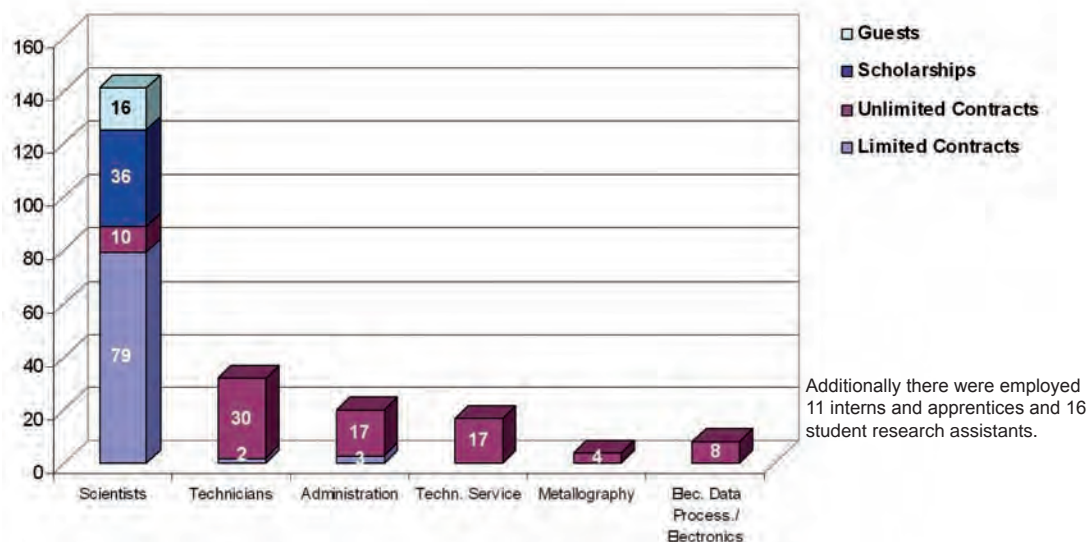- Interface Chemistry and Surface Engineering
- Computational Materials Design

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
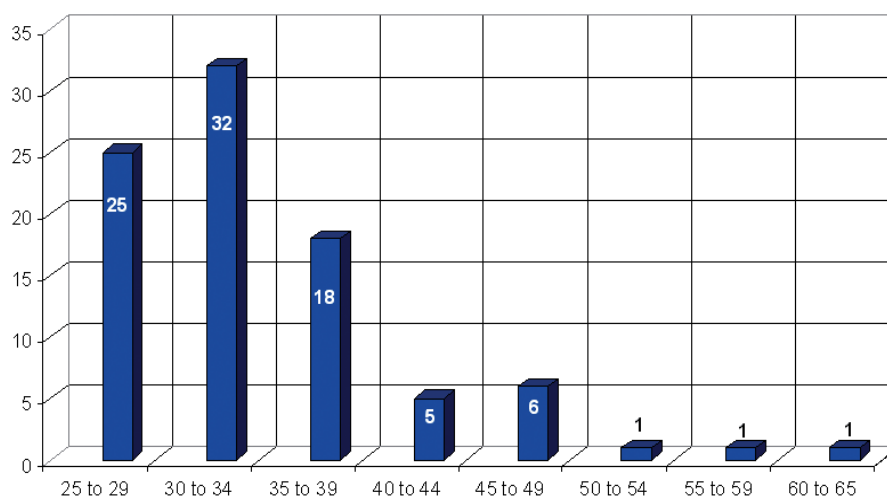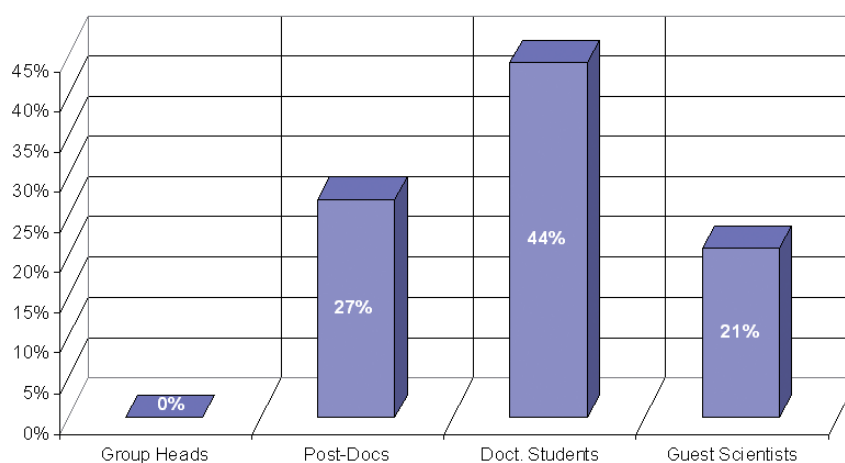EU: European Union

Personnel Structure

Number of Occupied Scientific / Non-Scientific Positions
(Dec. 2010, estimated)

Additionally there were employed 11 interns and apprentices and 16 student research assistants.

Age Distribution of Scientists
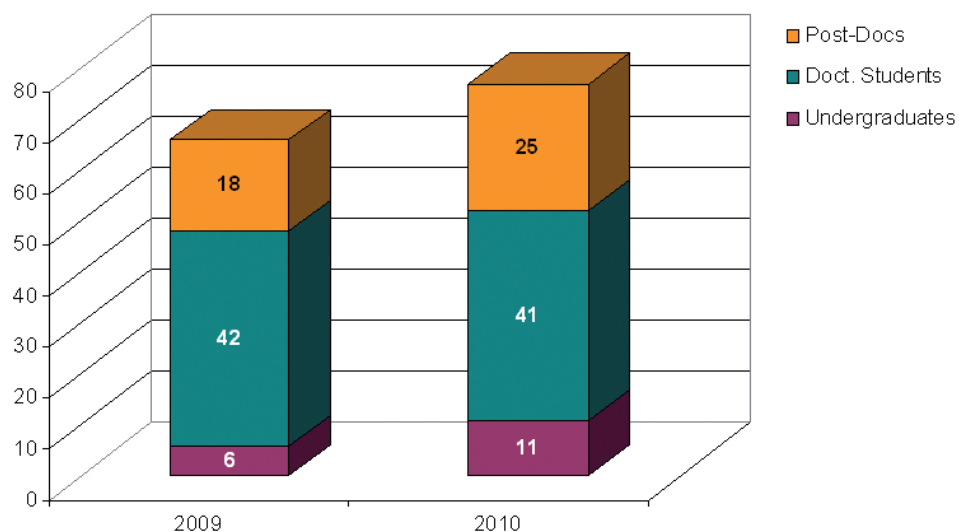(Dec. 2010, estimated)

Female Scientists
(Dec. 2010, estimated, percentual numbers)

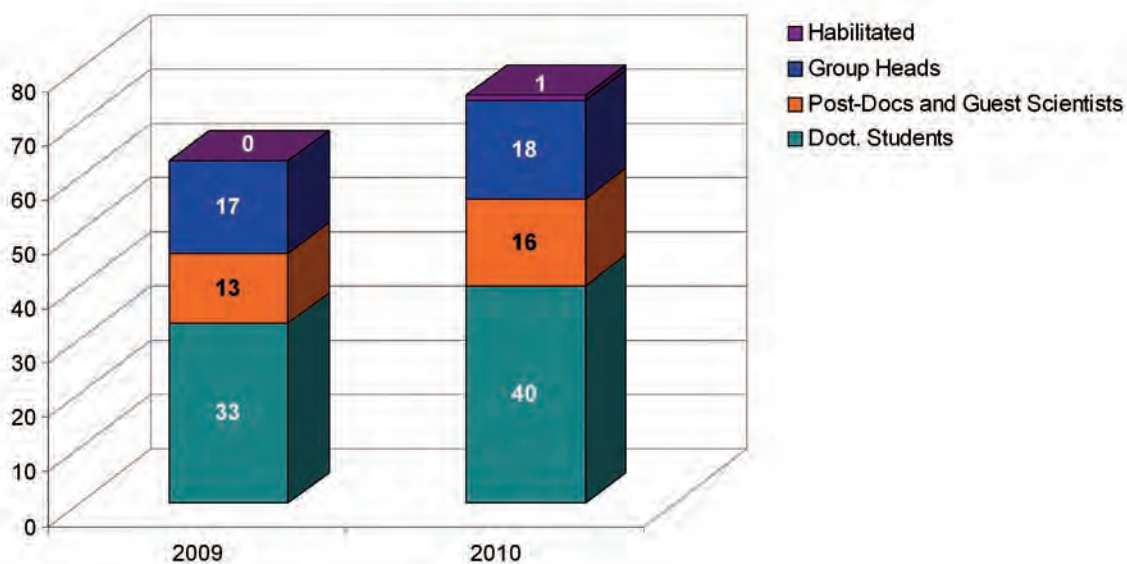## Number of Junior Scientists Financed via Third-Party Funds
(year 2010 data estimated)

Legend:
- Post-Docs
- Doct. Students
- Undergraduates

Number of Junior Scientists not Financed via Third-Party Funds
(year 2010 data estimated)

Legend:
- Habilitated
- Group Heads
- Post-Docs and Guest Scientists
- Doct. Students

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Employees and their Home Countries
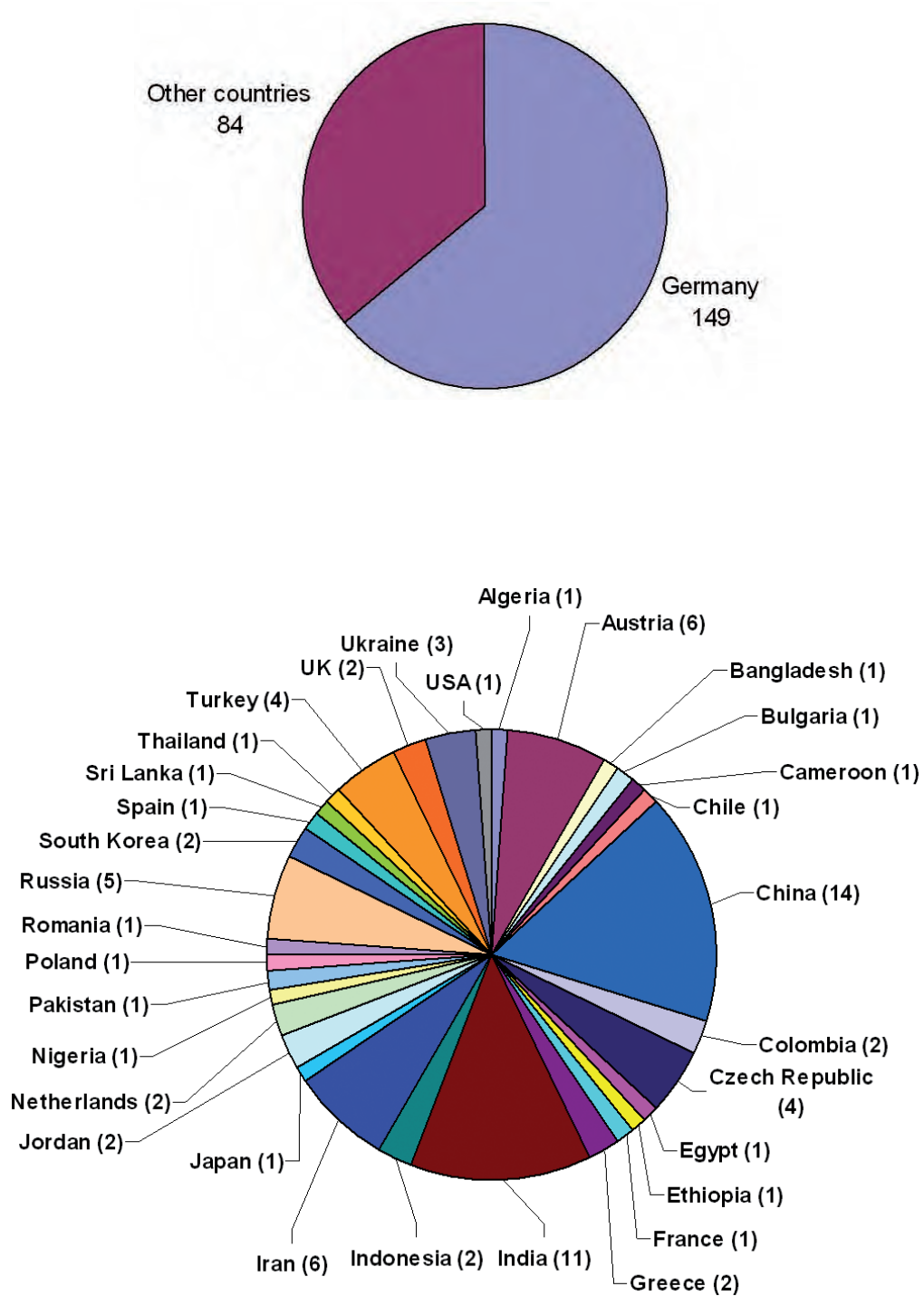
The Institute in Public

Much Ado about Iron: The Institute in Public

R. Loschen, C. Tamura

Research Coordination Office

Since September 2009 the Public Relations of the Institute have been restructured. With the establishment of the Research Coordination Office (RCO) all issues concerning public relations, internal and external communication and event management have been merged in one working unit. The Research Coordinator Rebekka Loschen is head of the Office, Claudia Tamura is assistant for public relations, Elke Gattermann on the other hand for the IMPRS-SurMat. Although the manpower has been reduced compared to the time before, the number of press releases, articles and public events could be significantly increased to more than 100 for the years 2009 and 2010. In the following we would like to give a short overview on the most important events of public relevance. An extract of the list of most important articles is given below.

Fig. 1: *Dr. Pyuck-Pa Choi, group leader for the in Germany unique 3D Atom Probe Tomography and key-note speaker at the opening ceremony in September 2009.*

In June 2009 Udo Brüx and the MPIE were awarded the prize for steel innovation under the patronage of the managing shareholder of Miele & Cie. KG and by the President of the Stahl-Informations-Zentrum, Prof. Dr.–Ing. Karl-Ulrich Köhler for the development of highly ductile light-weight TRIPLEX steels. Newspapers and local press reported on this high honour award on several occasions [1-7].

In September 2009 the newly established lab for 3D atom probe tomography in the department of Dierk Raabe was solemnly inaugurated. Raabe and Pyuck-Pa Choi, head of the new group, organised a scientific workshop to which experts contributed from all over the world (Fig. 1) [8-11].

In April 2010 for the first time a Federal Minister of Science and Education, Prof. Annette Schavan, came to visit the Institute [12-15]. At that time CEO, Martin Stratmann, explained the very unique role of the MPIE, between basic and applied industry research (Fig. 2). After an extended guided tour Schavan, a theologian by training, showed herself deeply impressed not only by the laboratories, but also by the enthusiasm of the scientists [16-20].

Some of the scientists of the MPIE have been awarded honours and prizes of international relevance: Otto-Hahn-Medal for Markus Valtiner, Willi-Korf-Award for Stefanie Sandlöbes or the Volker-Heine-Prize for Christoph Freysoldt, [21-23], just to name a few (Fig. 3). Additionally Dierk Raabe was nominated into the German Science Council, who advises the government for issues of science and higher education [24-26].

On September 4th 2010 the MPIE opened its doors to the public for the first time. The Stahl-Zentrum together with the MPIE had successfully applied in the competition: "365 Orte im Land der Ideen" (365 places in the country of ideas) [27]. On this occasion an open day was organised with many experiments presented by members of the MPIE. Families, students, the Lord Mayor of

Fig. 2: *Prof. Martin Stratmann (right) and Dr. Patrick Keil (left) explain the Ultra High Vacuum cluster to the Federal Minister of Science and Education, Prof. Annette Schavan.*

Fig. 3: *Prof. Volker Heine (right) when assigning the Volker-Heine Young Investigator Award to Dr. Christoph Freysoldt (left) during the* Ψ_k conference *in September 2010.*

Düsseldorf and many other interested people could e.g. watch a 3D molecule movie, see the forging hammer in progress or join on a journey into steel. More than 1500 people were impressed by various exciting presentations [28-48]. It became clear that events like this help to enthuse people about the wonders of science, especially children and young students showed considerable interest. Such events are thus a useful means for the recruitment of young scientists (Fig. 4). This is why the management has already decided to repeatedly organise open days in the future.

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2. Mitarbeiter-Information Stahl-Zentrum: „Stahl-Innovationspreis für MPIE", 15.07.2009.

3. RP Rheinische Post: „Innovationen aus Stahl", 12.11.2009.

4. RP Rheinische Post: „Düsseldorfer gewinnt Stahl-Innovationspreis", 01.07.2009.

5. RP Rheinische Post: „Spuren eines vergessenen Künstlers", 02.07.2009.

6. Stahl-Informations-Zentrum: „Hochmanganhaltige TRIPLEX-Leichtbaustähle", 01.07.2009.

Fig. 4: *Many children participated in the Kid's lab during the open day on September 4th, 2010. They learned basic principles of chromatography, ph-values and cold-rolling of fake-steel (modeling clay).*

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8. Focus Rostfrei: „Stahl in 3D - MPI für Eisenforschung weiht neues High-tech Analysengerät ein, 05.10.2009.

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11. Stahlmarkt: „Stahl in 3-D - Neues Hightech-Analysengerät eingeweiht", 05.05.2010.

12. WZ Westdeutsche Zeitung: „Forschungsministerin besucht Eisen-Forscher", 27.04.2010.

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16. RP Rheinische Post: „Ministerin Schavan bei Eisenforschern", 30.04.2010.

17. Stahlreport: „Ministerin besucht Max-Planck-Institut für Eisenforschung", 01.05.2010.

18. Elektrowärme International: „Ministerin Prof. Dr. Schavan besucht Max-Planck-Institut für Eisenforschung", 24.06.2010.

19. Stahl und Eisen: „Forschungsministerin Schavan im Max-Planck-Institut für Eisenforschung", 17.05.2010.

20. Mitarbeiter-Information Stahl-Zentrum: „Ministerin Schavan besucht Stahl-Forschung in Düsseldorf", 02.07.2010.

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23. Stahl und Eisen: „Warum wir Mitglieder im Stahlinstitut VDEh sind", 15.08.2010.

24. Steel-Research: „MPIE: Dierk Raabe in Wissenschaftsrat berufen", 15.05.2010.

25. RP Rheinische Post: „Neue Mitglieder in der Akademie der Wissenschaften", 15.05.2010.

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28. blechnet.com: „Tag der offenen Tür im Stahl-Zentrum", 10.02.2010.

29. Draht: „Tag der offenen Tür im Stahl-Zentrum", 10.02.2010.

30. Umformtechnik: „Tag der offenen Tür im Stahl-Zentrum Düsseldorf",   01.03.2010.

31. RP Rheinische Post: „Zentrum des Stahlinstituts VDEh zeigt seine Arbeit", 05.03.2010.

32. blechnet.com: „Tag der offenen Tür im Stahl-Zentrum", 23.03.2010.

33. maschinenmarkt.de: „Tag der offenen Tür im Stahl-Zentrum", 23.03.2010.

34. Metallhandwerk: „Tag der offenen Tür im Stahl- Zentrum", 10.05.2010.

35. Stahlmarkt: „VDEh-Jubiläum und Tag der offenen Tür", 01.06.2010.

36. Deutsches Verbände Forum: „Faszination Stahlforschung - Tag der offenen Tür", 04.09.2010.

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