PART I.

THE INSTITUTE

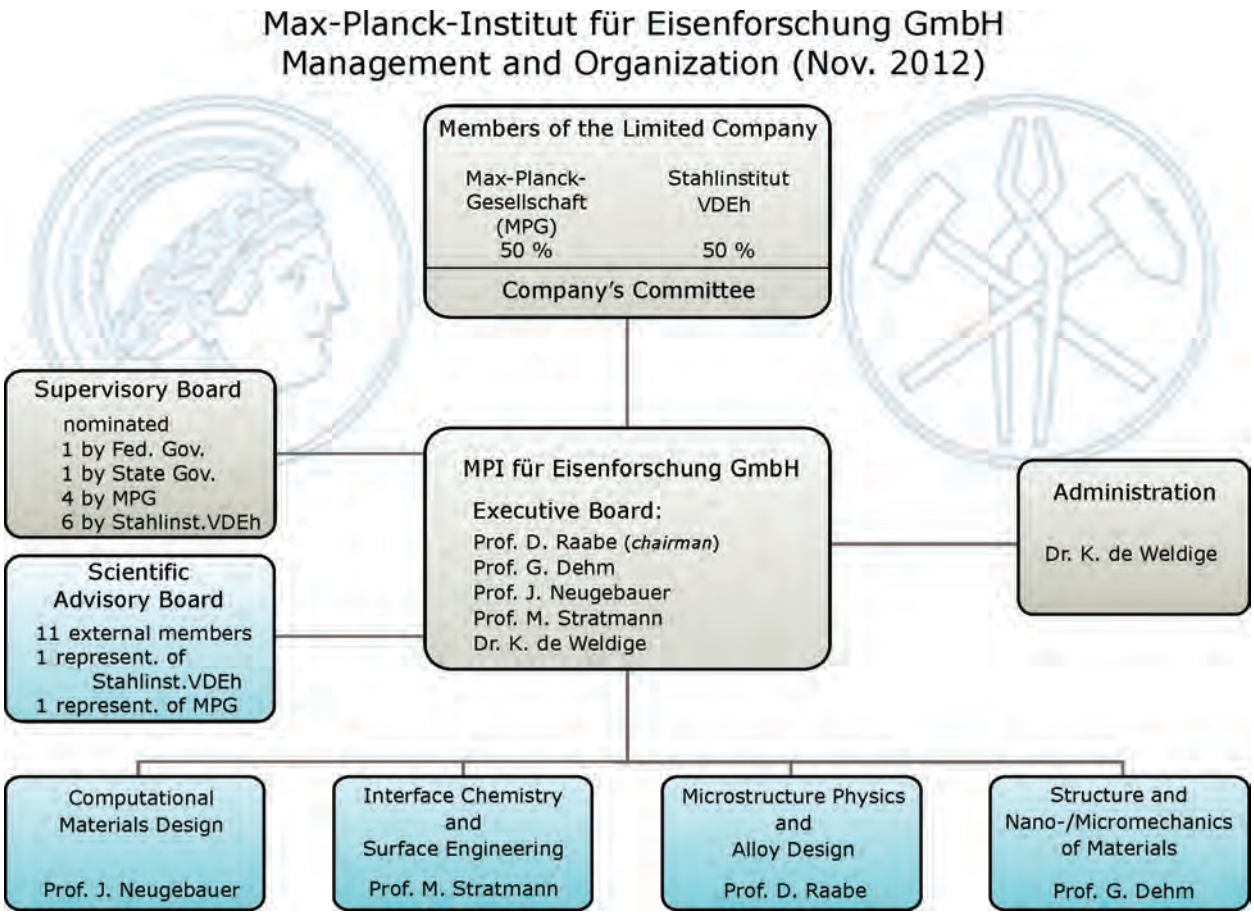
Management of the Institute

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

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

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

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



Scientific Organization

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

The institute is divided into the following departments:

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

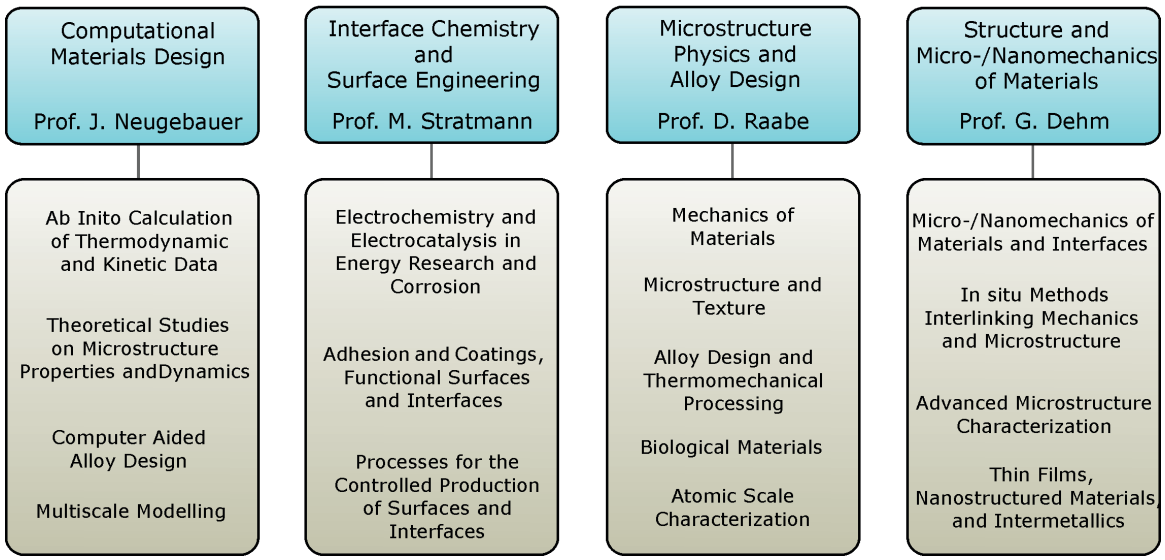
The main scopes of the departments are summarized in the figure below.

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

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

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

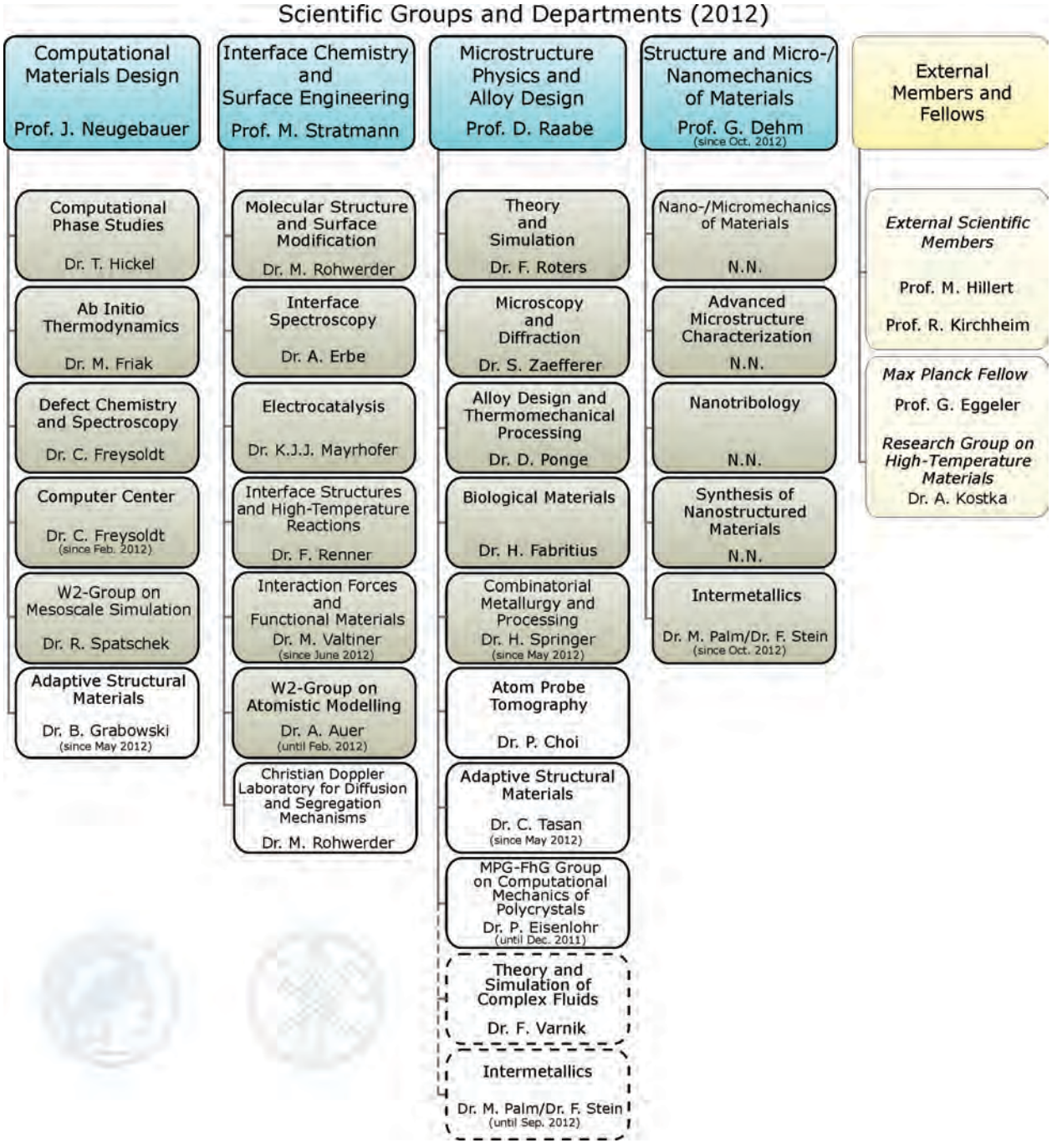
Scientific Scopes of the Departments



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

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

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



Recent Developments

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

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

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

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

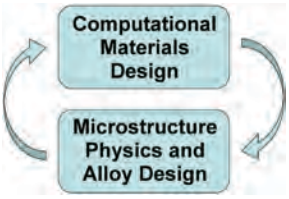
In May 2012 a research group on "Adaptive Structural Materials" started with the aim to develop next-generation high-strength and high-ductility metallic materials. A unique feature of the group is that it is headed by two heads, an experimentalist (C. Tasan) and a theoretician (B. Grabowski), thus ideally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

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

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

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

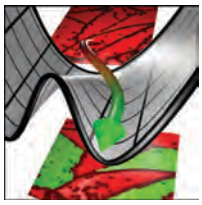
New Research Groups



Adaptive Structural Materials

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

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



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

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

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

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

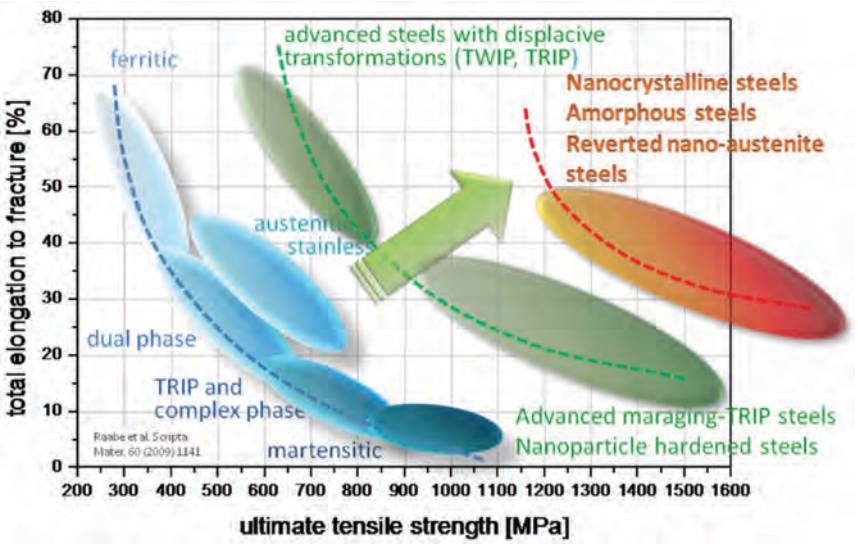


Fig. 1: *Inverse strength-ductility relation characterizing metallic alloys: Composition and microstructure changes make the material mechanically stronger but often reduce its ductility (elongation to failure). A major aim of the ASM group is to explore new design routes that shift the limit to the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

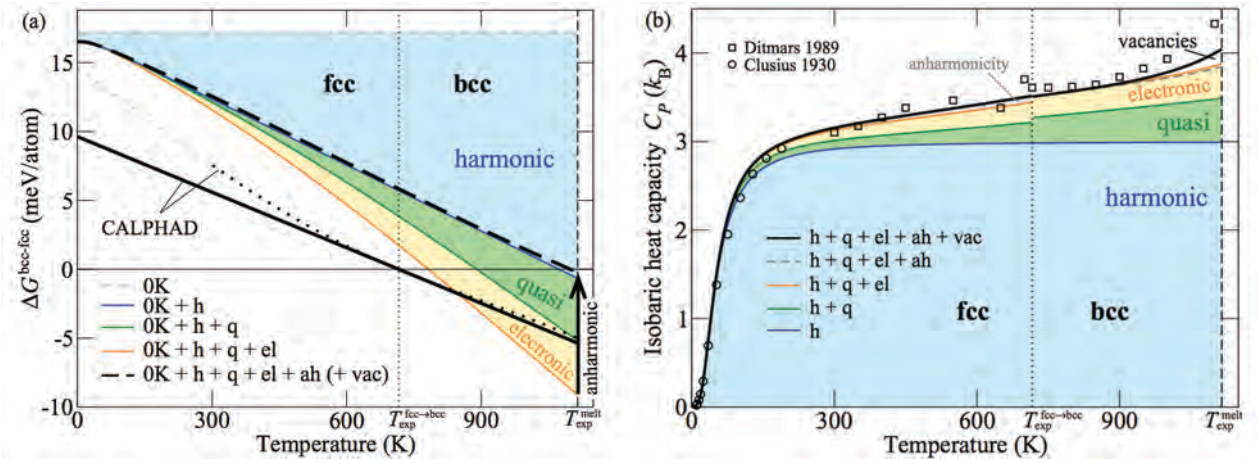


Fig. 2. *Importance of T>0 K contributions for the example of Ca. (a) Gibbs free energy difference between bcc and fcc. Only upon inclusion of all excitation mechanisms [(quasi)harmonic + electronic + anharmonic + vacancies] the correct T dependence is predicted (compare the slope of the dashed black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

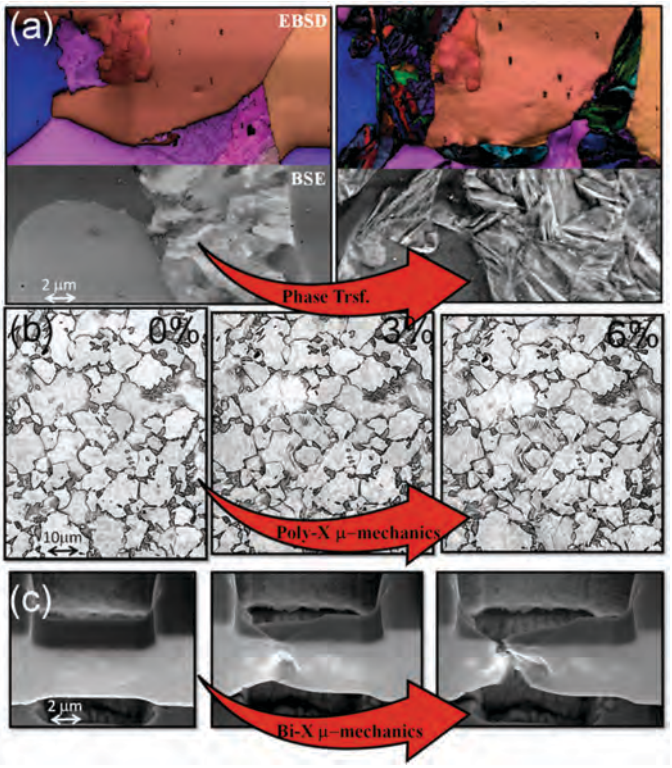


Fig. 3: *Results obtained using the novel experimental techniques employed in Adaptive Structural Materials group: (a) Tracking the same microstructural region through dual phase steel heat treatments: inverse pole figure and backscattered electron image of the start (pearlite-ferrite) and intercritically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

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

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

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

Combinatorial Metallurgy and Processing

Group Head: H. Springer

Department of Microstructure Physics and Alloy Design

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

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

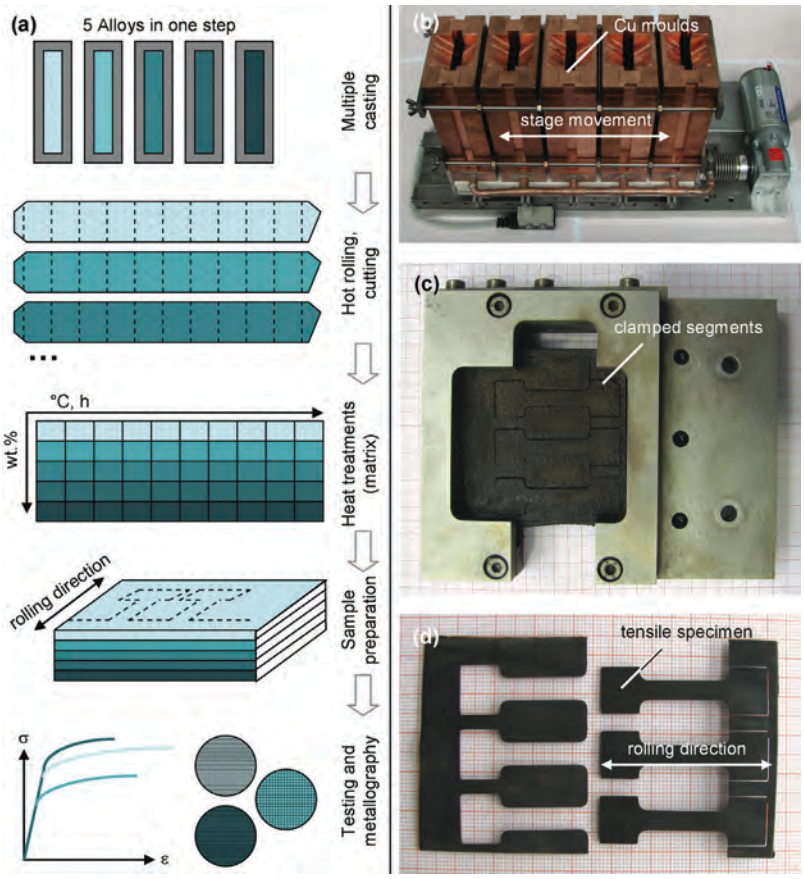


Illustration of the sample production process for Rapid Alloy Prototyping (RAP): (a) Schematic sketch of the RAP approach where the differently shaded colours refer to the different chemical compositions, (b) device for casting five alloys into separate Cu-moulds placed on a linear stage, (c) five segments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

References

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Interaction Forces and Functional Materials

Group Head: M. Valtiner

Department of Interface Chemistry and Surface Engineering

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

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

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

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

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

References

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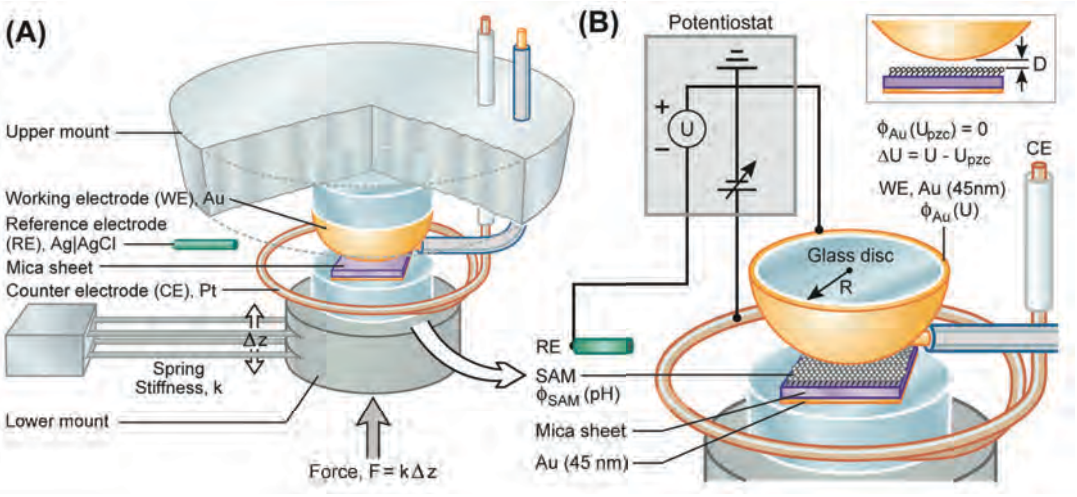


(A) Schematic of the EC-SFA. (B) Close-up of the experimental system. In this setup we apply an external electrochemical potential to an electrode (in this case Au, any metal can be used) and measure the ensuing force distance curves or friction forces due to lateral sliding. During experiments, the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

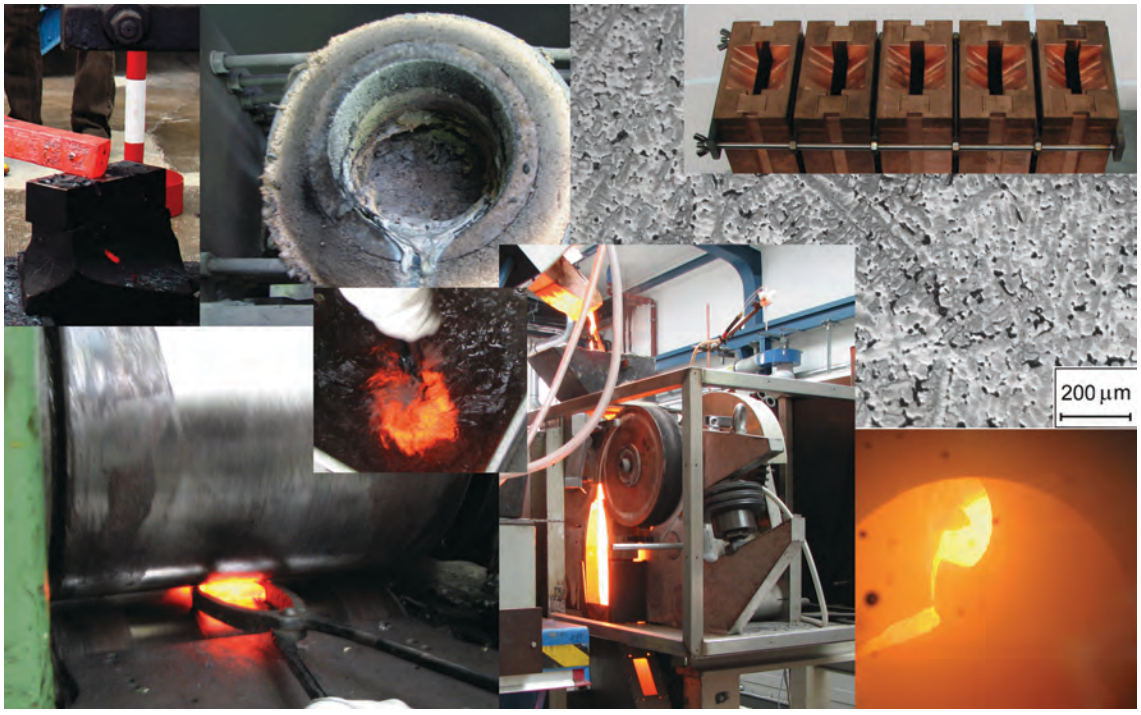
New Scientific Laboratories and Facilities

Metallurgy and Processing Laboratory

H. Springer

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

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



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

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

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

The (electrochemical) conversion of CO_2 into energy carriers like methane or methanol, as well as valuable chemicals such as ethylene, belongs to the modern "dream reactions" [1]. The fundamentals as well as the applied aspects of this reaction will be investigated in a dedicated laboratory in the Department of Interface Chemistry and Surface Engineering supported by the BMBF ($ECCO_2$, Kz: 01RC1101A). The approach, which will lead to an improvement of the understanding of the underlying processes and in consequence to the design of efficient catalyst materials, is particularly based on the development of advanced techniques coupling high-throughput electrochemistry with online product analysis [2].

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

References

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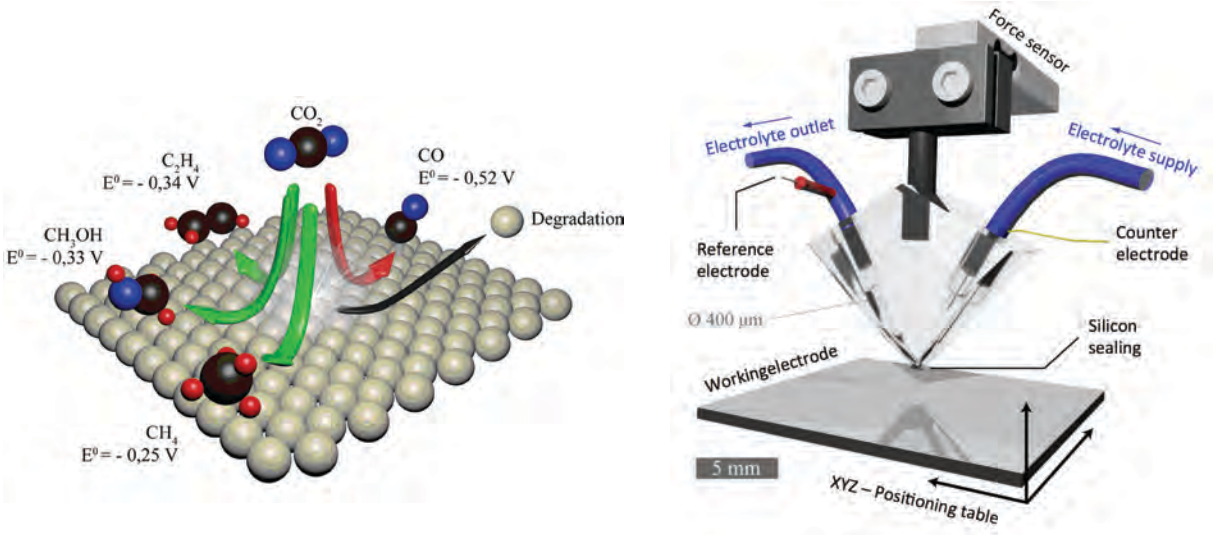


Scheme of the possible CO_2 reduction products including their standard potentials (left), and the scanning flow cell used for the electrochemical high-throughput screening investigations (right) [2].

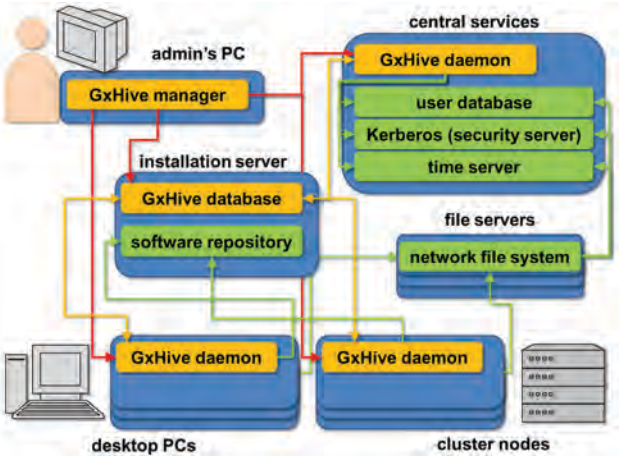
The GxHive Cluster Administration Package

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

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

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

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



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

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

Large-Scaled and Networking Projects

The International Max Planck Research School for Surface and Interface Engineering in Advanced Materials: Second Period Is Running Successfully

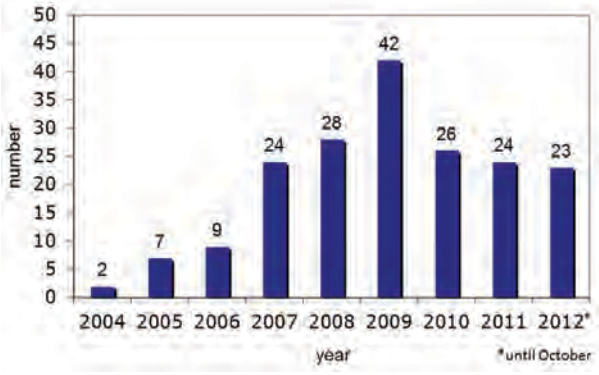
E. Gattermann, A. Erbe

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

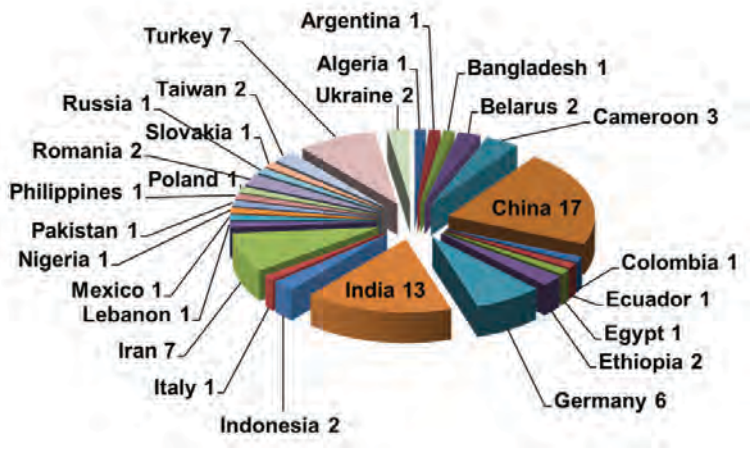
Organization. The SurMat board consists of five professors who decide upon the direction of the school. The two spokespersons of the IMPRS-SurMat are Martin Stratmann (MPIE) and Gunther Eggeler (RUB). The coordination of the IMPRS-SurMat is managed at the MPIE. Andreas Erbe remains scientific director,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

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

Number of SurMat students.



Number of publications by SurMat students in peer reviewed journals.



Origin of SurMat students by countries.

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

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

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

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

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

Center for Electrochemical Sciences

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

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

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

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

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

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

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

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

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

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

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

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Interdisciplinary Centre for Advanced Materials Simulation – ICAMS

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

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

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

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

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

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

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

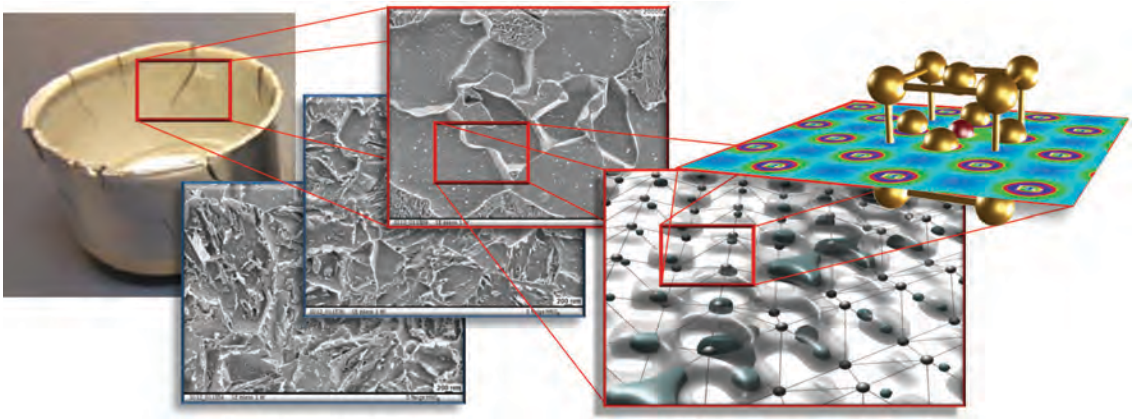
Hydrogen Sensitivity of Different Advanced High Strength Microstructures (HYDRAMICROS): An International Research Consortium

T. Hickel, R. Nazarov, J. Neugebauer

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

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

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



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

SMARTMET: Adaptive Nanostructures in Next Generation Metallic Materials

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

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

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

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

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

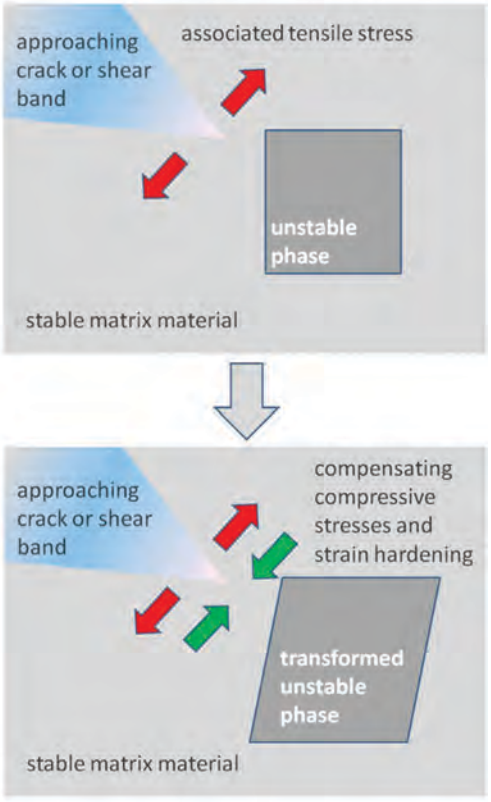


Fig. 1: Mechanical *response of an unstable second phase embedded in an otherwise stable matrix on an approaching load. In the schematic case depicted the transformation is associated with a volume change and shear. The resulting local stress field upon transformation of the unstable phase can stop localization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

The European Union's Seventh Framework Programme for Research and Technological Development

ERC Advanced Research Grant SMARTMET

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

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

In 2007 the Max-Planck-Institute in Düsseldorf (MPIE) and RWTH Aachen University jointly initiated a collaborative research center (Sonderforschungsbereich, SFB 761) on the quantum mechanics guided design of new Fe-based materials. The initiative is funded by the German Research Foundation (Deutsche Forschungsgemeinschaft DFG). Speaker and chairman of the project is Prof. Wolfgang Bleck (Institute of Ferrous Metallurgy, RWTH Aachen University) and vice-chairman is Prof. Dierk Raabe (MPIE). The first four year phase of the SFB 761 ended in June 2011. The results were successfully presented during the evaluation of the SFB in early 2011. Based on this evaluation and the written report a second four year phase was granted by the DFG.

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

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

Inspired by the success of the first period, SFB 761 will continue in the manufacturing and characterization of Fe−Mn−Al−C-steels of different compositions, the use of *ab initio* methods for the prediction of key thermodynamic parameters (relevant, e.g., for TWIP, TRIP, weight reduction, shear band formation and kappa-carbide formation), and the quantification of the effects of chemical composition, strain rate and temperature on the occurrence and interaction of different strengthening mechanisms. The long-term perspective lies in the development of predictive and quantitative multiscale models of materials and processes that are based on *ab initio* simulations and the establishment of a new class of structural steels based on the Fe−Mn−C system.

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

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

Cluster of Excellence RESOLV

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

*Ruhr-Universität Bochum (RUB)

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

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

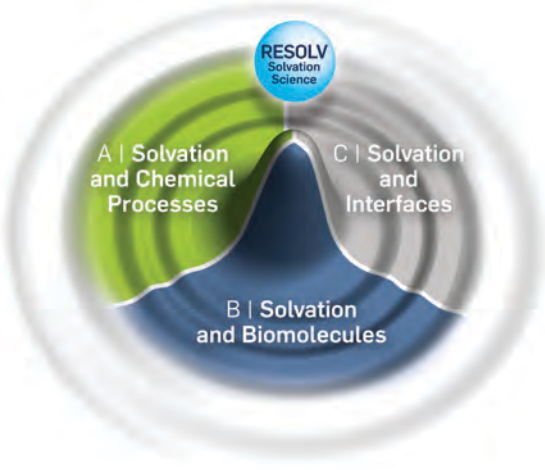
RESOLV represents a new stage in the cooperation between three universities and four leading non-university institutions in the Metropolis Ruhr: RUB, Technische Universität Dortmund, Universität Duisburg-Essen; Fraunhofer-Institut für Umwelt-Sicherheits- und Energietechnik (UMSICHT); MPI für Chemische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

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

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

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

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



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

MAX-PLANCK-GESELLSCHAFT

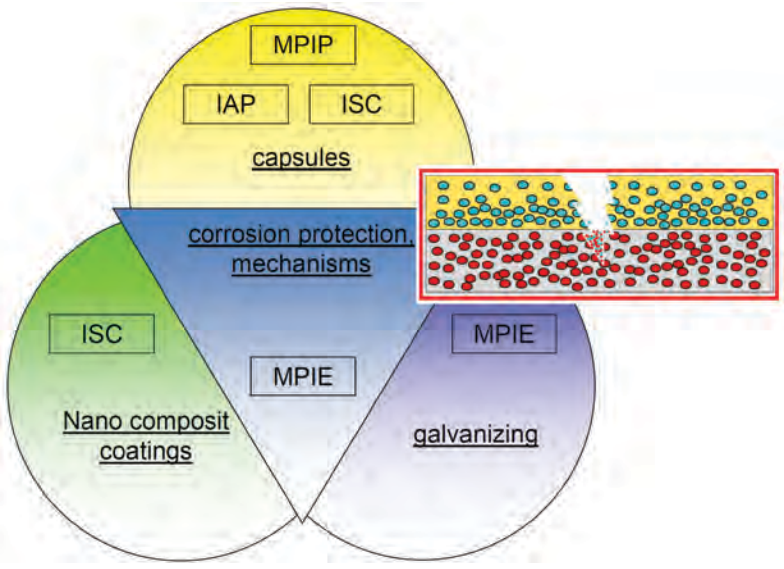
Cooperation between Max Planck Society and Fraunhofer Society:

Fraunhofer

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

M. Rohwerder

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



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

Northern Alliance for Competence (Kompetenzverbund Nord, KVN) –

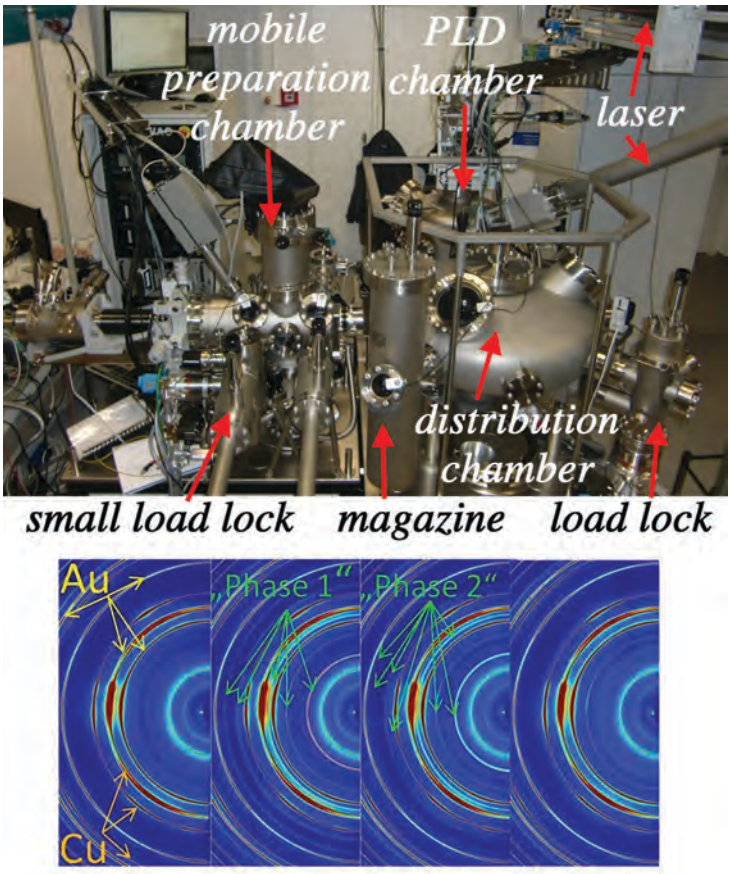
German Research Priorities in Electrochemistry with the Focus on Electromobility:

Studies on Model Interfaces for Li Ion Batteries

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

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

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



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

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

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

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

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

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

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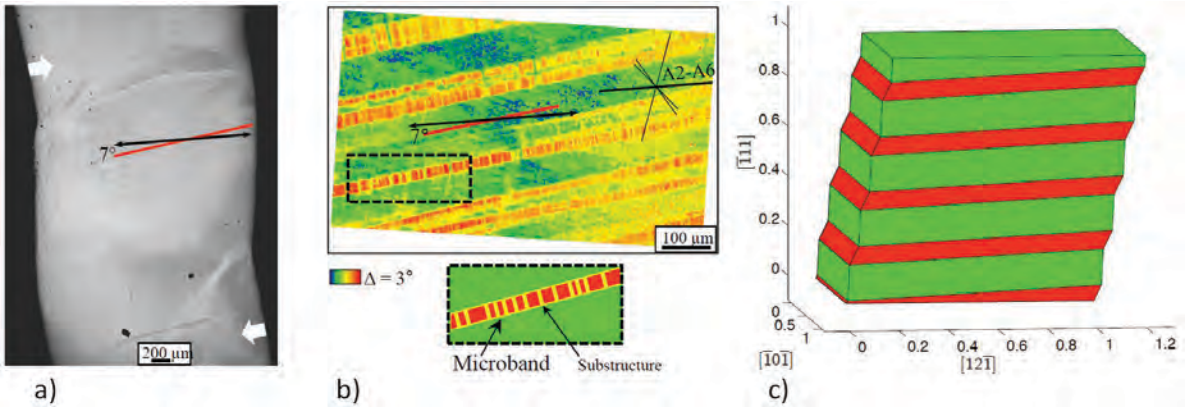


a) SEM micrograph of a shear deformed copper single crystal. The direction of load is indicated by white arrows. b) EBSD map of a deformed area which shows the crystallographic orientation changes within 3°. Occurrence of microbands (red areas) is observed. Within the microbands, formation of a local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

Aachen Institute for Advanced Study in Computational Engineering Science – AICES

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

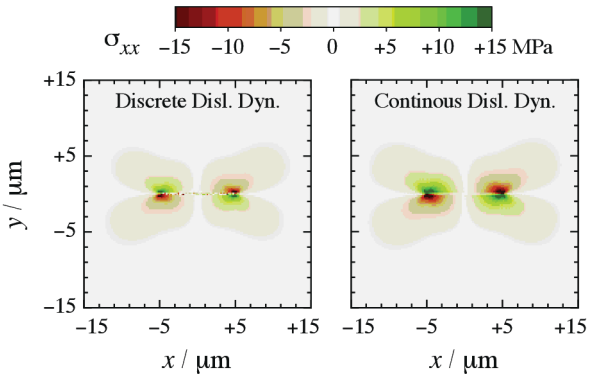
Introduction. The Aachen Institute for Advanced Study in Computational Engineering Science (AICES) is a graduate school that has been established within the framework of the Excellence Initiative of the German federal and state governments in 2006. In 2012 AICES was successful in securing funding from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

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

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

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

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



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

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

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

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

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

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

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

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