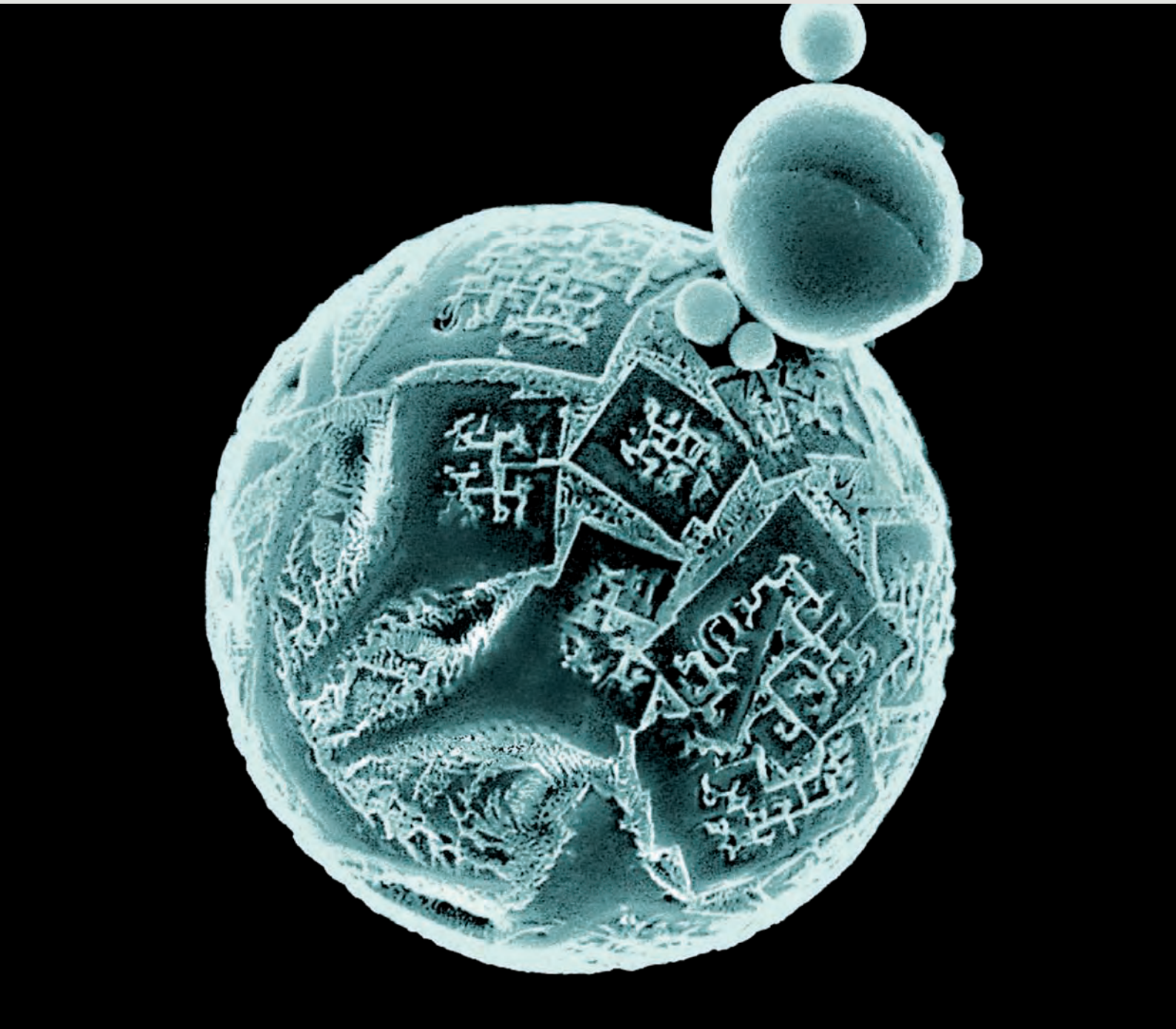
MAX-PLANCK-GESELLSCHAFT

Scientific Report 2005 / 2006

Max-Planck-Institut
für Eisenforschung GmbH



Max-Planck-Institut für Eisenforschung GmbH

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December 2006
Max-Planck-Institut für Eisenforschung GmbH
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Germany

Front cover

The SEM image reveals the morphology of melt-atomized and rapidly solidified eutectic iron-boron powder particles with composition Fe – 4wt.%B which experienced extremely high cooling rates of the order of $5 \cdot 10^4$ to $5 \cdot 10^5$ K/s by quenching in an argon inert gas jet. The small satellite particles of less than 3µm in size are in the amorphous state and have the composition $Fe_{80}B_{20}$. The „coarser" powder particle consists of primarily solidified metastable borides Fe_3B surrounded by a fine-grained eutectic of α iron and Fe_3B borides. The metastable Fe_3B crystals possess the orthorhombic $D0_{11}$ or tetragonal $D0_e$ crystal structures as determined by X-ray diffraction. In the centre of the borides the retained eutectic reveals a „Chinese script" microstructure.

Imprint

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PREFACE

This report is part of a series summarising the scientific performance of the Max-Planck-Institut für Eisenforschung. In particular, this volume covers the years 2005 and 2006. However, as this Scientific Report is also part of a Status Report presented to the President of the Max Planck Society every 6 years, the overviews of the departmental work given in *Part II* also include additional information on the years 2001 to 2004.

Over the period of 6 years the institute has undergone a tremendous change. Nearly all of the existing scientific groups have been newly established and because of the ongoing major reconstruction of the institute all laboratories can be regarded as new. Most importantly, two of the directors, namely, Jörg Neugebauer and Anke Pyzalla have taken up their research in Düsseldorf during the last two years.

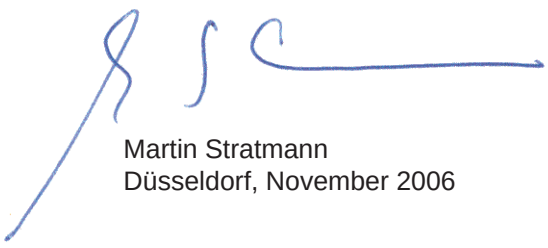
As a result the scientific structure of the institute now differs largely from the period before 2000. Traditionally the institute has been divided into classical areas like metallurgy, forming, physical metallurgy, materials technology and surface properties. Today this traditional scheme has been given up. For instance a department for conventional metallurgy does not exist anymore and the department of materials technology will cease to exist at the end of 2008. The remaining departments have established a network-like structure with strong horizontal links. Each department has a strong scientific focus in itself, such as microstructures and mesoscopic modelling in the department of Dierk Raabe, ab-initio modelling in the department of Jörg Neugebauer, X-ray, neutron and synchrotron radiation based analytical techniques as diffraction and scattering in the department of Anke Pyzalla, and surface and interface science in the department of Martin Stratmann. In addition to these mainly departmental initiatives additional areas of common interest establish strong links between the departments. Each of these inter-departmental research fields is coordinated by one of the department heads. The areas are *New Structural Materials* (Anke Pyzalla), *Microstructure-Related Materials Properties* (Dierk Raabe), *Stability of Surfaces and Interfaces* (Martin Stratmann) and *Scale-Bridging Simulation of Materials* (Jörg Neugebauer). The institute is convinced that this matrix-like structure stimulates cooperation between the departments and furthermore is the adequate structure for the development and characterisation of new structural materials which in fact is the main focus of the institute's mission. It is expected that after fully establishing all departments this kind of interaction will dominate the institute's daily life.

This report consists of four parts:

- *Part I* deals with the organization of the institute including a short section on the recent developments as well as brief descriptions of the large-scaled and networking projects, outstanding laboratories and the central facilities of the institute.

- *Part II* and *Part III* cover the research activities of the institute splitted into two parts. Part II gives a description of the departmental work and Part III contains selected papers which summarise major scientific achievements in the above mentioned four areas of common interest of the institute.

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



Martin Stratmann
Düsseldorf, November 2006

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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.

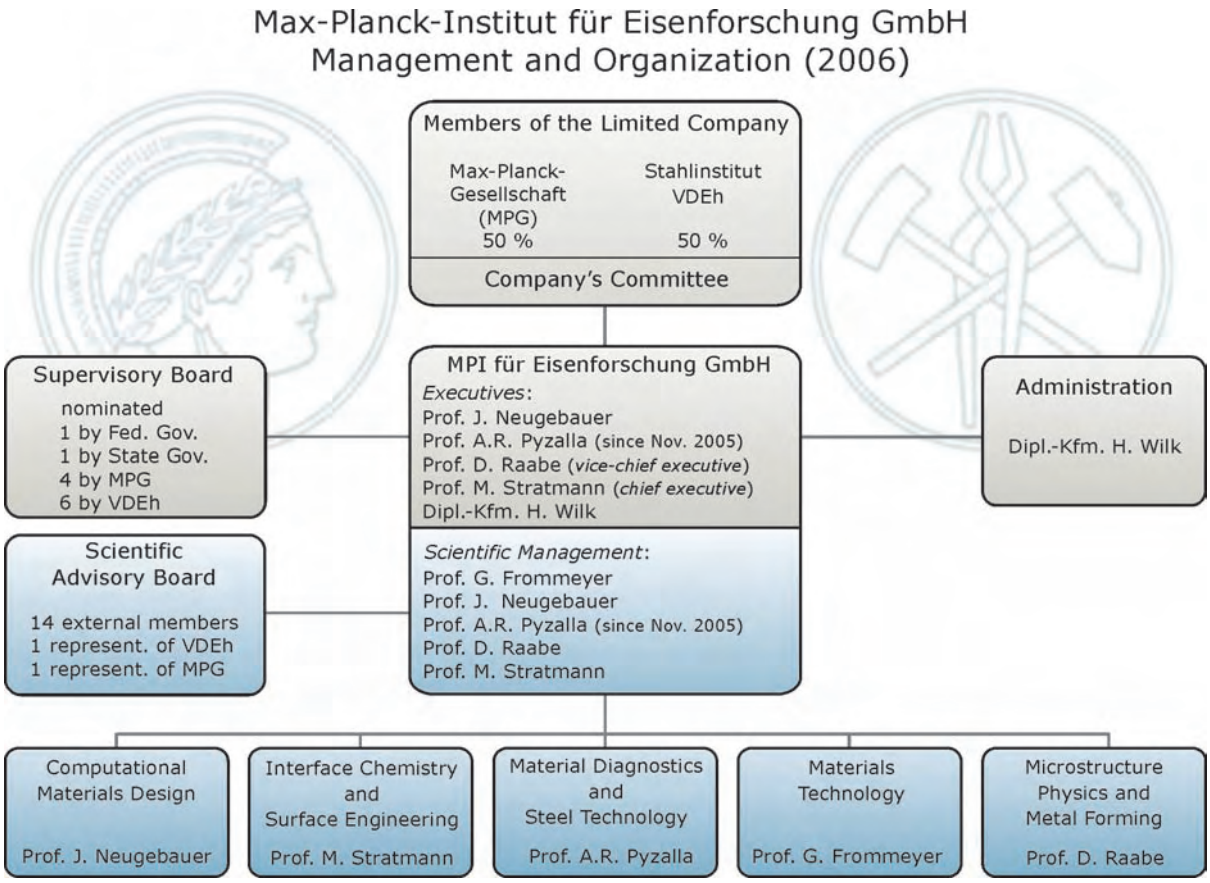
The institute was founded in 1917 by the Verein Deutscher Eisenhüttenleute (VDEh) and incorporated into the Kaiser Wilhelm Gesellschaft, the predecessor of the Max Planck Society. The institute was first located in Aachen and was associated with the Technical University of Aachen. The institute later moved in 1934/35 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 incorporated into the Max Planck Society. The institute rapidly expanded and new laboratory buildings were erected in the early 1960s. Following the appointment of H.J. Engell as director in 1971, a complete reorganization of the institute was carried out. Up to 2002, the institute was headed by a chief executive director (1971-1990: Prof. Engell, 1990-2002: Prof. Neumann) and an associated administrative director.

Since 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 institution'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 finding the right balance between 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. Nearly 100 employees on permanent positions including scientists, technicians and administrative staff are working at the institute, and an additional 100 scientists are financially supported through third party funds and scholarships.

Since 2000, the institute is again under reconstruction. While currently the third stage of reconstruction is running (see also p. 12 'Recent Developments'), the renovations are expected to be completed in 2008.



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 characterisation and properties.

In November 2005, Prof. A.R. Pyzalla became a new director at the MPIE and established a Department on Material Diagnostics and Steel Technology. In July 2005, the Department on Metallurgy and Process Technology, which was provisionally headed by Dr. Büchner up to that time, was closed. Now, the institute is organized into the five following departments:

- *Computational Materials Design* (Prof. J. Neugebauer, since Nov. 2004): description of materials properties and processing based on ab initio (parameter free) multiscale simulation techniques

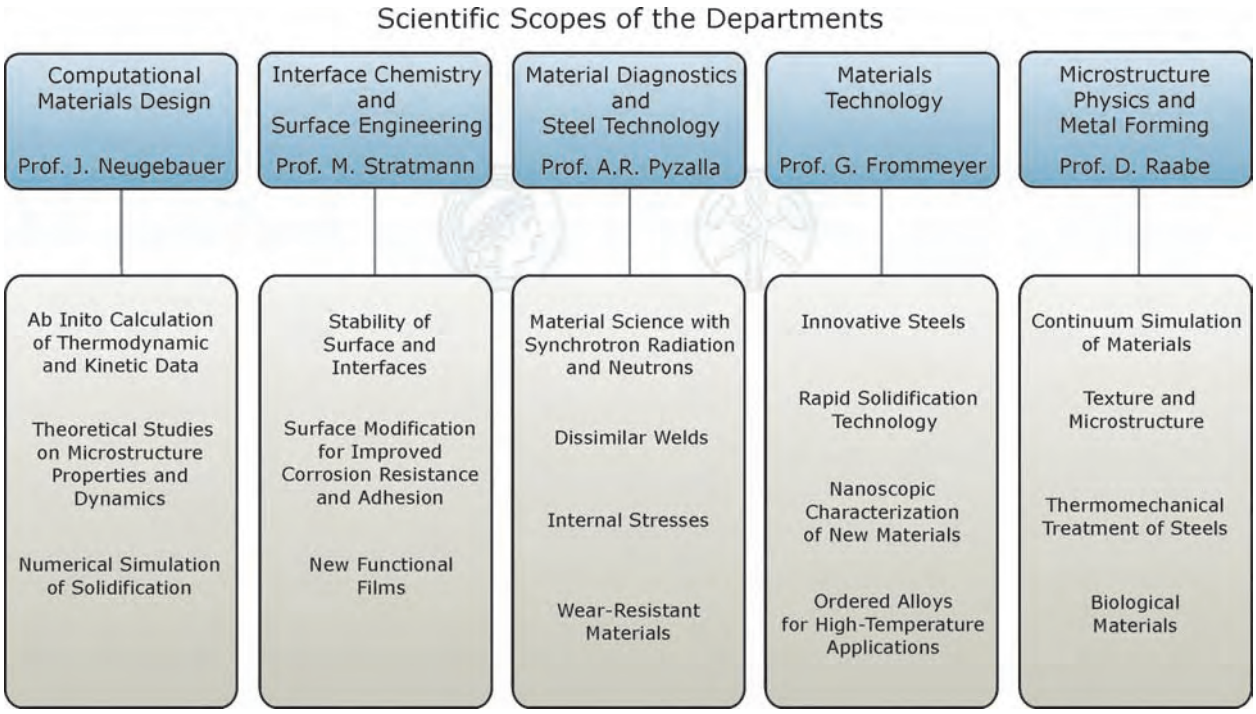
- *Interface Chemistry and Surface Engineering* (Prof. M. Stratmann): aspects of environmentally accelerated degradation of surfaces and interfaces like corrosion and deadhesion and the engineering of new and stable surfaces and interfaces

- *Material Diagnostics and Steel Technology* (Prof. A.R. Pyzalla, since Nov. 2005): microstructure - residual stress - property relations using e.g. electron microscopy, synchrotron and neutron diffraction, tomography and scattering.

- *Materials Technology* (Prof. G. Frommeyer): novel lightweight steels, new intermetallic materials and rapid solidification processes

- *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 broken down into research groups which are typically managed by group heads. The figure below 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 contrast to the other parts of the report, it covers the years 2001-2006.

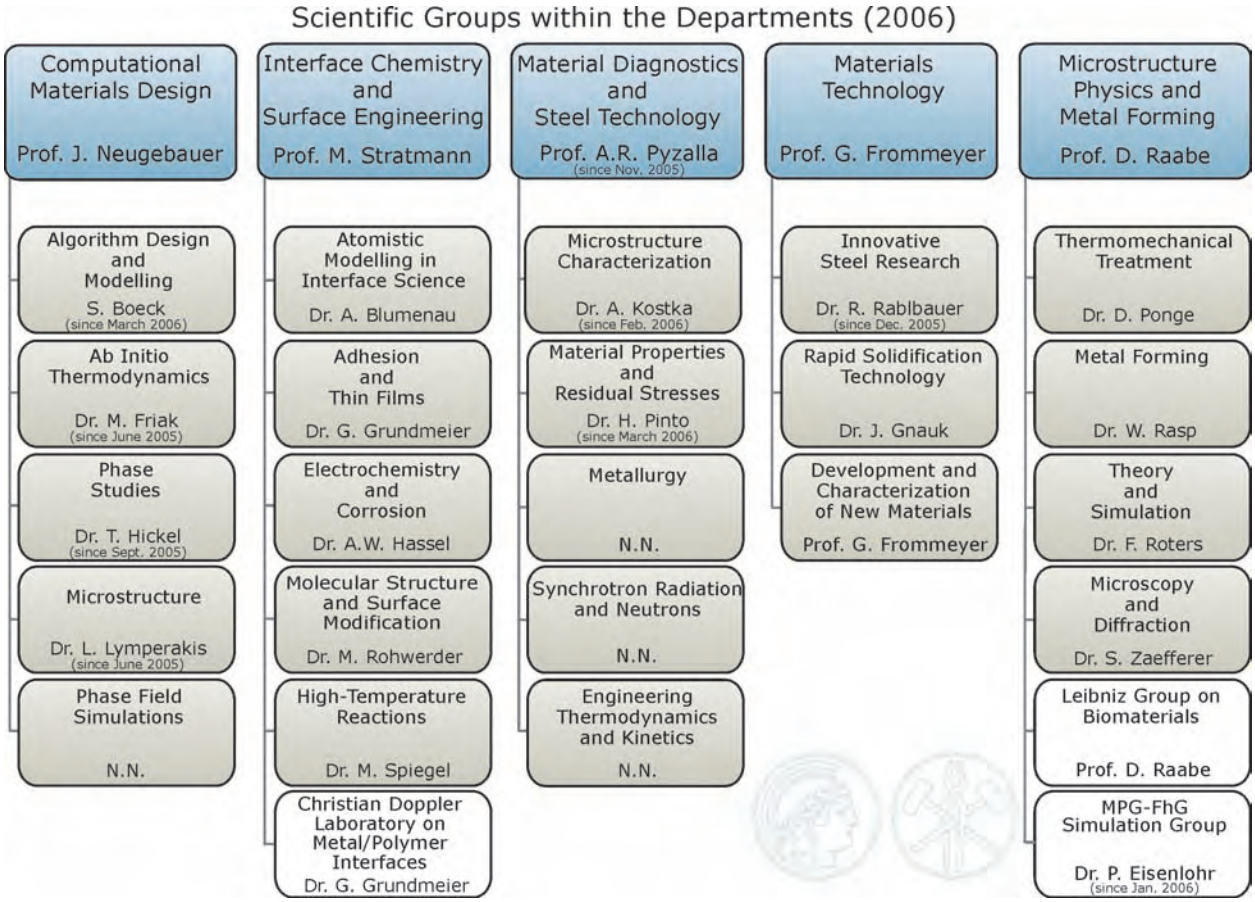
In addition to departmental research, certain research activities are of common interest within the institute. These central research areas are highly interdisciplinary and combine the experimental and theoretical expertise available from within the different departments in order to achieve a scientific and technological breakthrough in highly competitive areas of research. 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

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

The research within the institute is therefore 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.



Recent Developments

The last two years have been characterized by the appointment of two new directors, Prof. Dr. Jörg Neugebauer and Prof. Dr. Anke Pyzalla, who initiated the new departments „Computational Materials Design“ (CM) and „Material Diagnostics and Steel Technology“ (WS). With these appointments the restructuring and the new scientific orientation of the institute, which started in 1999 with the appointments of Prof. Dr. D. Raabe and Prof. Dr. M. Stratmann, has been successfully completed.

Prof. Dr. Jörg Neugebauer accepted the appointment in Nov. 2004 and started the department in May 2005. The department opened the new and rapidly emerging field of parameter-free (ab initio) atomistic simulation of complex materials to the institute. The CM department consists presently of four groups. The computational tools which are and will be developed and applied by the department allow to accurately calculate and predict materials properties and processes solely on the computer, i.e., without the need of experimental data or empirical fitting parameters. By employing multiscale techniques, i.e., combining the ab initio tools with mesoscopic and/or macroscopic concepts such as thermodynamics, kinetics, elastic theory or statistical mechanics, the department addresses a wide range of topics related to steel and metallic alloys. Examples are the calculation of phase diagrams, tailoring alloys with predefined mechanical properties or the study of formation, evolution and properties of grain and phase boundaries, extended defects etc. The bottom up approach of the CM department nicely complements the top down simulation approach (i.e. refining macroscale approaches such as finite element modeling by adding mesoscale concepts) which is already well established in the institute.

Prof. Anke Pyzalla accepted the appointment to become a director at the institute on Nov. 1, 2005 and started in Jan. 2006 with organizing the department „Material Diagnostics and Technology of Steels“. The objective of the department is the microscopic characterization of engineering material microstructures and their load-induced changes. The characterization will be performed by developing and employing state-of-the-art techniques in diffraction, scattering, and tomography using neutron or synchrotron radiation. These techniques will be used to understand the relation between microstructure and properties and between microstructural changes and damage under complex loading conditions. The methods allow covering the whole length scale between interatomic distances to industrial components. In its final stage the department will consist of five working groups.

The combination of the activities of the already existing and the new departments significantly expanded the scientific profile and width of the institute and allowed new links and projects with various academic and industrial research institutions. Prominent examples are the Max-Planck Multiscale Materials Modeling (MMM) initiative initiated by our institute with Prof. D. Raabe as speaker, the Joint Max-Planck-Fraunhofer Initiative on Computational Mechanics of Polycrystals (CMC^n), the Inter-Institutional Max Planck Research Initiative ‘The Nature of Laves Phases’, and the initiative to establish an international centre of advanced materials simulation (ICAMS) which will be established at the Ruhr Universität Bochum with a budget of approximately 25 Mio € for the next 5 years.

Another important issue for the institute has been the ongoing reconstruction of the institute buildings, which has started in 2000. In the last two years the reconstruction has largely progressed. Hall 8 has been finished and is in use since May 2005. In hall 9 new offices have been constructed for the department of Prof. A. Pyzalla and are in use since May 2006. Lab spaces in hall 9 are still under construction and are planned to be finished in Feb. 2007. The design of laboratories for microscopy, e.g. a new TEM, has started. The reconstruction of the „Blue Building“, where offices and the high performance computer centre for the CM department of Prof. J. Neugebauer will be accommodated, will be started in spring 2007 and is expected to be finished in spring/summer 2008.

Large-Scaled and Networking Projects

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

Introduction. In 1999, the Max Planck Society together with the Association of Universities and Other Education Institutions in Germany launched an initiative to promote junior scientists called the International Max Planck Research Schools. In the winter semester 2000/2001, the first Research Schools were started as cooperative efforts involving Max Planck Institutes together with German and foreign universities and research facilities. These Schools offer outstanding students from Germany and abroad the possibility to prepare for their PhD exam in a structured programme providing excellent research conditions.

IMPRS-SurMat. The application for the IMPRS for Surface and Interface Engineering in Advanced Materials (IMPRS-SurMat) was considered and granted by a scientific commission of the Max Planck Society in January 2003. It is a collaborative project involving the Max-Planck-Institut für Eisenforschung in Düsseldorf, the Max Planck Institute for Coal Research in Mülheim/Ruhr, and four engineering and sciences departments of the Ruhr University in Bochum. The Max-Planck-Institut für Eisenforschung takes over the lead management. In addition to the aforementioned German partners Prof. Tian Zhongqun and Prof. Lin Changjian from the State Key Laboratory for Physical Chemistry of Solid Surfaces (PCOSS), Xiamen University, Prof. Mao Weimin from the Department of Materials, University of Science and Technology, Beijing, and Prof. Zhao Dongyuan from the Department of Chemistry, Fudan University are involved in this Research School. In autumn 2006 Prof. Neugebauer and Prof. Pyzalla from the Max-Planck-Institut für Eisenforschung and Prof. Schuhmann from the Chemistry department of the Ruhr University have been accepted as new colleagues and supervisors within the IMPRS-SurMat.

Opening ceremony. To emphasize the importance of the IMPRS-SurMat a great opening ceremony took place on December, 17th, 2004. At this opportunity the concept of the Research School has been presented as an instrument for the promotion of young scientists and furthermore as a place of scientific and cultural exchange to the public and to our invited guests. The doctoral students which have been accepted to the Research School in its first year of existence were officially awarded their scholarships by high-ranking representatives of our financial partners from industry, from the government of North Rhine-Westphalia, the Max Planck Society and the Ruhr University in Bochum.

Meeting of all IMPRS-SurMat students on the occasion of a status seminar in spring 2006.

Scientific focus and teaching programme. The main research objective is to correlate the chemical structure, morphology and mechanical properties of heterogeneous surfaces and buried interfaces with functional properties of the materials and to optimize them by means of advanced surface modification techniques.

Within the framework of a structured PhD programme the doctoral students have to attend special lectures in addition to their research work. Most of the SurMat students grew up in different educational systems with different methods of teaching and a deviating scientific focus. Furthermore they graduated in different subjects and already obtained a high degree of specialisation during their Master thesis work. Therefore, a special teaching programme is essential for providing them with a sound knowledge base and to enable them to efficiently work and communicate in an international scientific environment with interdisciplinary research topics.

The lectures, which have exclusively been conceived for this purpose, are combined into four units. Each unit lasts two weeks and consists of five different lectures. The lectures focus on the physical chemistry of surfaces and interfaces, phase transformations induced by the presence of interfaces and the mechanical properties of interface-dominated materials, thin films, and nano-scale patterning and processing of thin film-covered materials. Topics include corrosion, adhesion, tribology, catalysis, and the physical properties of thin functional layers. All courses take place during four subsequent semesters in spring and autumn each year. The participation in those courses is compulsory. At the end of each course the students have to pass a written exam. The individual results are certified and summarised in a final IMPRS certificate. In February 2005 the teaching programme started with the unit T1, and in October 2006 the fourth and last teaching unit T4 has been completed by the first generation of SurMat students. From spring 2007 the series of lectures will start again. All lectures have been included in the university calendar of the Ruhr University Bochum. The school is open for external PhD students, too, which have not been admitted to the IMPRS-SurMat. The number of participants is limited and a registration is required.

In addition to their scientific work and the teaching programme the SurMat students have the opportunity to learn German during their stay in Germany. In cooperation with the “Institute for International Communication (IIK e.V.) and the University Language Centre (USZ) of the Heinrich Heine University in Düsseldorf the Max-Planck-Institut für Eisenforschung offers German language training from the beginners level up to very advanced levels (Oberstufenniveau).

External sources of scholarships. As a supplement of the scholarships regularly financed by the basic budget of our Research School, German companies financially support the SurMat. Since 2004 the ThyssenKrupp Stahl AG covers the costs of two scholarships, the Salzgitter AG contributed one scholarship. Since 2006 the Chemetall GmbH donated another scholarship. Each of those scholarships has been granted according to the regulations of the Max Planck Society for the Advancement of Science for a maximum duration of three years.

Status quo. Students are admitted to the International Max Planck Research School for Surface and Interface Engineering in Advanced Materials twice per year in spring and autumn. Since the official start of the IMPRS-SurMat in 2004 about 800 students from more than 60 nations applied for a PhD position. The distribution of applicants referring to their home countries is characteristic and comparable to that of other IMPRS in Germany with a similar scientific focus. About 70 % of all applicants come from the following five countries: India (40 %), China (12 %), Pakistan (8 %), Iran (6 %) and Romania (5 %). The proportion of female applicants relating to the total number of applicants is about 20 %, the proportion of the admitted female PhD students in SurMat is even higher – about 30 %. Meanwhile 25 IMPRS-SurMat students and 3 affiliated students from 17 nations have been admitted to the IMPRS-SurMat. The acceptance ratio is below 5 %. In 2007 the first students will successfully complete the structured PhD programme of the IMPRS-SurMat and will be conferred a Max Planck Certificate and a PhD or Doctoral degree.

Outlook. An international conference/workshop on surface and interface engineering will take place at the end of 2006, almost two years after the official opening ceremony. In 2007 the main task will be to intensify the selective advertising e.g. in high ranking South and Middle American universities in cooperation with other IMPRS. Especially the organization of an IMPRS PhD fair has been discussed during 2006.

Triple-M – Max Planck Initiative on Multiscale Materials Modeling of Condensed Matter

D. Raabe, J. Neugebauer

Introduction. In September 2006 the Max Planck society has launched a new integrated project on the theory of solid matter. The title of the initiative is "Triple-M – Max Planck Initiative on Multiscale Materials Modeling of Condensed Matter". The project is designed as an interdisciplinary theory initiative among 6 Max Planck institutes.

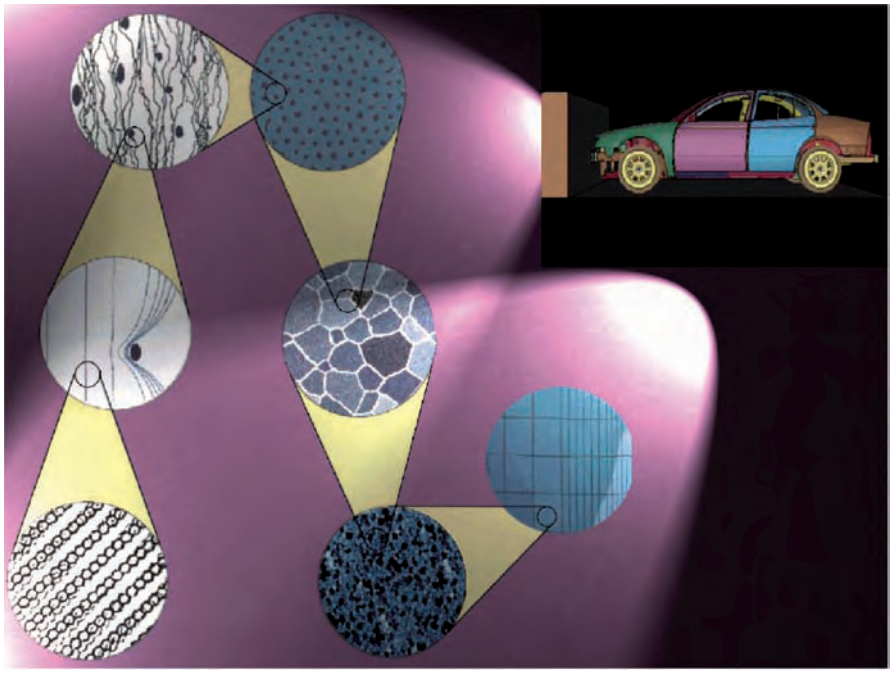
The project aims at combining existing and newly emerging theoretical approaches to bridge time and space scales in the modeling of condensed matter phenomena in the field of materials science. Besides this scientific goal the project will develop the interaction among the condensed matter theory groups of the Max Planck Society with the goal to establish a center of expertise. The joint theory activities in that center will lead to the creation of new interdisciplinary approaches with respect to both the theoretical methods and the underlying materials physics investigated. Also the initiative will serve other groups to utilize the existing and new theory competence in that field.

The principal investigators during the first three years of the project are Professor Dr. Martin Jansen (MPI for solid state research), Professor Dr. Kurt Kremer (MPI for polymer research), Professor Dr. Stefan Müller (MPI for mathematics in the natural sciences), Professor Dr. Jörg Neugebauer (MPI für Eisenforschung), Professor Dr. Dierk Raabe who is the initiator and speaker of the initiative (MPI für Eisenforschung), Professor Dr. Matthias Scheffler (Fritz-Haber institute), Professor Dr. Walter Thiel (MPI for coal research), and Dr. Karsten Reuter (Fritz-Haber institute).

Details of the MMM initiative. Research on many condensed matter phenomena requires understanding of the underlying thermodynamics and kinetics at multiple length and time scales spanning many orders of magnitude as a rule (from Ångstroms to meters; from picoseconds to years).

A grand challenge in computational materials science is to combine these vastly different time and length scales and crosslink the knowledge and the theoretical schools from the different scale ends.

Traditionally, research in that field has developed during the last 15 years with a focus on theoretical methods that are particularly applicable and at the same time confined to certain scale regimes. Typical examples at very small scales are the various electronic structure methods (QM-methods, density functional theory). Above that scale molecular dynamics based on empirical potentials and atomic scale Metropolis Monte Carlo models are widely used. At the mesoscopic scale different rate theoretical methods are in use which typically mimic ground states or dynamical properties in a statistical fashion (Master equations, Langevin equations). Also



Schematical presentation of some scale transitions encountered in the field of multiscale materials modeling.

automaton-type lattice models (Potts Monte Carlo lattice models, cellular automata) and pseudo-particle dynamical approaches are frequently applied at that scale. Finally, continuum-based thermodynamics or constitutive kinetic models which are typically solved using variational methods (phase field and finite element simulations) serve at the mesoscopic and macroscopic scales.

The most extreme differences in scale and also in modeling philosophy currently exist between electronic structure models and the continuum theory of condensed matter. In both fields tremendous progress is currently taking place: Due to the increase in computational power together with the advance of novel theoretical, mathematical, and numerical methodologies, there is a rapidly growing theoretical physics and theoretical chemistry community pursuing electronic-structure simulations. At the other end of the spectrum, mathematics, physics, and engineering have jointly made large progress in obtaining numerical solutions to sets of nonlinear partial differential equation systems which describe condensed matter phenomena on the basis of continuum models without resolving individual electrons or pseudo-particles. These various theory schools addressing fundamental problems in the field of computational materials science from different scale ends all exist within the Max-Planck Society and some of the participating groups are working in this field at the leading edge already for years. For instance, the groups of Martin Jansen (Stuttgart), Kurt Kremer (Mainz), Jörg Neugebauer (Düsseldorf), Matthias Scheffler (Berlin), and Walter Thiel (Mühlheim) have leading expertise in the fields of ab initio methods, pseudo particle dynamics, and statistical mechanics. The groups of Stefan Müller (Leipzig) and Dierk Raabe (Düsseldorf) are at the forefront of continuum theory of condensed matter.

The aim of this initiative is to bring together these groups with their respective expertise in condensed matter modeling to jointly develop novel theoretical methods for bridging the different time and length scales from the electron to the continuum theory of matter within the Max Planck Society for the first time.

A main goal is the development of modeling approaches which combine, wherever useful, the different scales and techniques. It is obvious in that context that it is not always pertinent or necessary to bridge *all* scales from the electron to the macroscopic scale for solving a certain problem rather than to focus on those scales which are of relevance for a given task.

Moreover, it is intended to bring together scientists with a strong background in condensed matter modeling from seemingly different areas such as physics, materials sciences, mathematics, chemistry, and biomaterials for a strongly interdisciplinary collaboration.

In condensed form this vision can be summarized into the following points which in particular explain the anticipated added value arising from the synergy of the collaboration of the different theory groups exceeding the already very strong individual activities of each of the groups alone:

1. No closed theory framework exists which unifies particle-based and continuum-based models providing smooth transitions between the two views of matter. Rendering one description into the other is one of the most challenging tasks in condensed matter theory.
2. Although some of the principal investigators have already tackled multiscale problems in the sense that 2 or 3 orders of space and time magnitude were covered in earlier projects the fundamental problems associated with scale-bridging simulations across much larger gaps in time and space have until today not been addressed. One example of such a problem is the challenge to arrive from electronic structure calculations via molecular dynamics at physically-based simulations of an automotive crash test or of a super heat resistant turbine design in a consistent theoretical framework. Another example would be to arrive from molecular simulations of biomolecules and biominerals at the macroscopic prediction of bone damage or blood vessel mechanics.
3. The integration of the different theory groups into one Max-Planck-Multiscale-Materials-Modeling Initiative will create a method- and competence-pool. Benefits from this center of competence are not only be expected for other condensed matter theory groups (inside and outside the Max Planck Society) but also for experimental groups which increasingly make use of modern modeling tools without having the necessary theoretical and computational background. The latter point is of large relevance since many experiments can nowadays no longer be fully analyzed or even basically understood without accompanying models owing to the complexity of the condensed matter phenomena inspected and boundary conditions imposed during the experiments.
4. Worldwide no center for the education of young scientists in the field of multiscale materials modeling exists covering all relevant theoretical and computational methods from ab initio to large scale finite element methods.
5. Materials of interest within the initiative are metals, ceramics, composites, semiconductors, as well as synthetic and biological soft matter.

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

F. Stein, O. Prymak, M. Palm, G. Frommeyer, D. Raabe

The project „The Nature of Laves Phases“ is an inter-institutional research initiative funded by the Max Planck Society since the beginning of 2006. Four Max Planck institutes, namely the

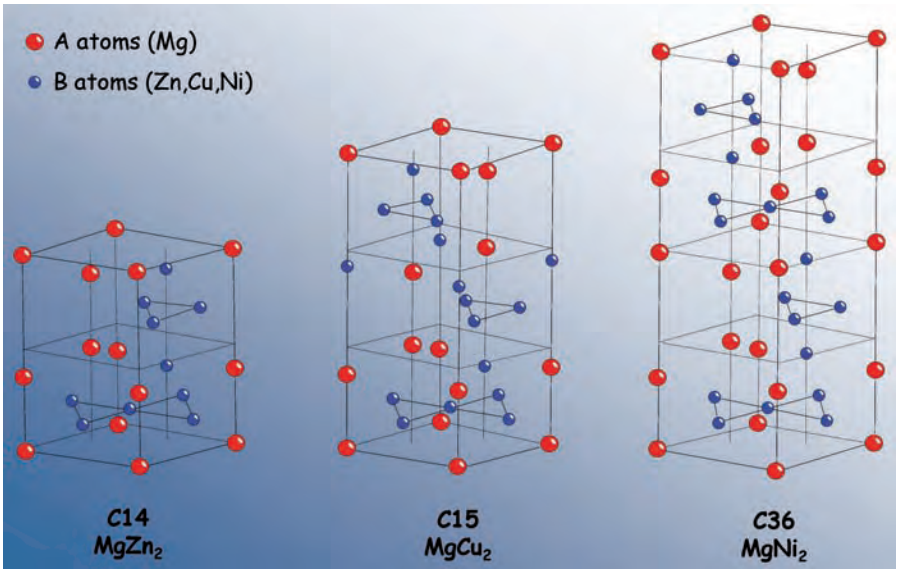
- Max Planck Institute for Chemical Physics of Solids (Prof. Y. Grin, Dr. G. Kreiner) in Dresden,
- Max Planck Institute for Metal Research (Prof. E.-J. Mittemeijer, Dr. A. Leineweber), in Stuttgart,
- Max Planck Institute for Solid State Research (Prof. M. Jansen, Dr. D. Fischer), in Stuttgart, and the
- Max-Planck-Institut für Eisenforschung GmbH,

are working in close co-operation within this research initiative in order to create a high-level forum with strong interdisciplinary character for the experimental and theoretical investigation of complex intermetallic phases. The joint scientific expertise and research equipment of the involved Max Planck research groups promise a break-through in the understanding of intermetallic phases ranging from atomic to mesoscopic phenomena. The scientific topic is comprehensive and includes synthesis of novel, high-melting phases, investigation of their thermodynamic stabilities and crystallographic structures, characterization of atomic and mesoscopic phenomena, quantum mechanical and thermodynamical modelling of the phases as well as studies of corresponding kinetic phenomena. The Laves phases, which form the largest group of intermetallic phases, are chosen as model systems. The physical metallurgy of the intermetallic phases is much more complex than that of other established alloys, but has to be understood in greater detail as theses phases are promising candidates for the design of new metallic materials with superior properties.

Laves phases received worldwide attention within the last years (e.g. [1-7]) as they have become candidates for several functional as well as structural applications. The most prominent example for the first group of applications is the utilization of Laves phases as hydrogen storage materials especially in nickel-metal hydride batteries on the basis of the Laves phase $Zr(V,Mn,Ni)_2$. Moreover, they are candidates for magnetoelastic transducers ($(Tb,Dy)Fe_2$) and show promising superconducting properties ($(Hf,Zr)V_2$). In view of structural applications, Laves phases are attractive because of their high strength up to high temperatures. The principal shortcoming is their pronounced brittleness at ambient temperatures which is being tried to overcome by combining Laves phases with a ductile phase.

Laves phases have the general formula AB_2 and can crystallize in three different structure types: the cubic $MgCu_2$ type (C15), the hexagonal $MgZn_2$ type (C14), and the hexagonal $MgNi_2$ type (C36). The crystallographic structures of the three polytypes are closely related as is visualised in Fig. 1. They differ only by the particular stacking of the same four-layered structural units. As a consequence of this close relationship, the differences in total energies between the polytypes are generally very small and in many transition metal systems, two or three Laves phase polytypes coexist in equilibrium showing temperature-, composition- and/or pressure-dependent transformations.

Geometric and electronic factors such as the atomic size ratio of the A and B atoms and their



Schematical presentation of the crystal structures of the three Laves phase polytypes in a hexagonal setting.

valence electron numbers are well known to affect the occurrence of a Laves phase and various simple models based on these factors have been developed aiming at a prediction of the stable polytype. In two recent review papers [8,9], we have critically assessed these factors and discussed some general features of the polytypism of Laves phases by comparing a large number of Laves phase-containing systems. It could clearly be shown that all the existing models and calculations fail in giving general predictions of the occurrence and structure type of Laves phases.

Some fundamental questions - many of them strongly correlated - concerning the nature of Laves phases have to be answered. This includes an explanation to the problem which binary systems form stable or metastable Laves phases, which phases are thermodynamic competitors and which Laves phase polytypes are thermodynamically stable or metastable. A very important issue concerns the frequent occurrence of extended homogeneity ranges of Laves phases in binary and ternary systems. Regarding this, the research initiative offers the opportunity of studying the factors which are determinant for the stabilization of intermetallic phases at non-stoichiometric compositions. Another fundamental problem which will be addressed by the research initiative is the understanding of the phase transformations between different polytypes: How does it proceed and what is the kinetics of such a phase transformation? It is also of very high importance to investigate the character of chemical bonding as a function of the components, composition, structure, temperature and pressure and to find out what the relation between physical and mechanical properties and real structures of the polytypes is.

The project „The Nature of Laves Phases“ focuses on the series of binary and ternary Laves phases-containing systems Nb-X and Nb-X-Al (X = Cr, Mn, Fe, Co) [10-16]. These systems were chosen as all three polytypes of Laves phases occur and in several cases the co-existence of two or even three Laves phase polytypes was observed within one system showing temperature- or composition-dependent transformations. Therefore, these systems offer an ideal opportunity to investigate the above basic questions.

The ultimate goal is the understanding of phase formation as a function of the components, composition, temperature and pressure as well as the influences of the processing of the materials on the final properties. In particular, the study of the interplay between crystal structure, chemical bonding and properties and a targeted development of novel metallic materials for demanding applications are of eminent importance. The research initiative is regarded as a nucleus for a long lasting collaboration in order to forge an international group of interest to achieve the above long-term objectives by understanding the model class of intermetallic compounds called Laves phases.

More detailed information on the research initiative „The Nature of Laves Phases“ can be found on the project website http://laves.mpie.de.

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Computational Mechanics of Polycrystals - CMC^n

P. Eisenlohr[+)], D. Raabe[+)], F. Roters[+)], L. Hantcherli[+)], P. Gumbsch[#)], H. Riedel[#)]

First Joint Research Group of Max Planck Society (Max-Planck-Institut für Eisenforschung, Düsseldorf [+)]) and Fraunhofer Society (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg [#)])

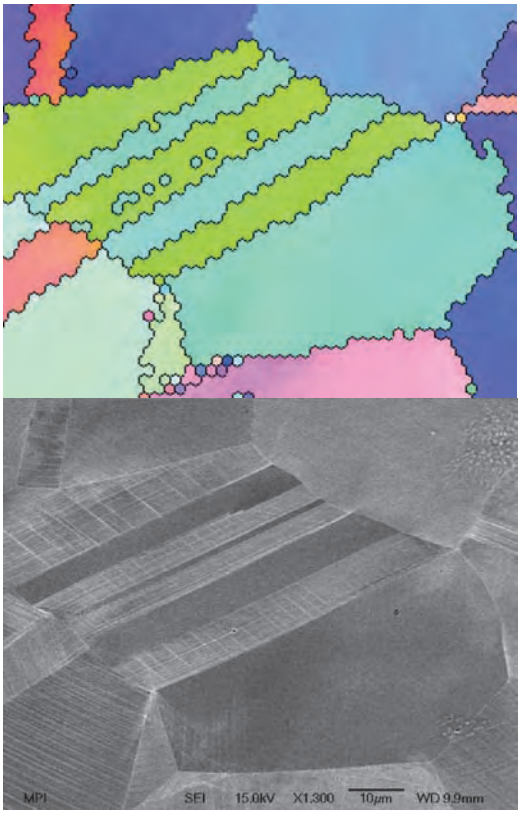
The new joint research initiative on Computational Mechanics of Polycrystals (CMC^n) which was established in October 2005 as the first ever joint research group between the Max Planck Society (Department of Microstructure Physics and Metal Forming at the Max-Planck-Institut für Eisenforschung, Düsseldorf) and the Fraunhofer Society (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg) pursues the idea to develop and enhance novel theoretical approaches for the field of mechanics of crystalline matter with the aim to promote its use for industrial applications such as encountered in the fields of aerospace, automotive, and medical engineering. Chief scientist and project leader of the initiative at the Max-Planck-Institut für Eisenforschung is Dr. P. Eisenlohr.

Initiators and speakers of the initiative are Prof. D. Raabe on behalf of the Max Planck Society and Prof. P. Gumbsch on behalf of the Fraunhofer Society.

The research field of crystal mechanics has gained substantial maturity during the last decade, which makes it an ideal candidate to prepare its exploitation as an advanced computational tool for industrially highly innovative and complex simulation problems. The field of crystal mechanics is highly interdisciplinary bringing together approaches from the metal physics of plastic deformation, plasticity-induced phase transformations, interface science, mathematics of non-linear partial differential equations, numerical mathematics, continuum mechanics, and forming technology.

The new group will deal with all relevant scientific and engineering challenges associated with crystal plasticity finite element simulations of the microstructure evolution and mechanical response of complex metallic materials. In terms of metal physics the group will particularly focus during the first 3 years period on the micromechanical fundamentals associated with multiphase mechanics, deformation induced phase transformations, twinning, size effects, and interface mechanics. In terms of the computational and engineering challenges associated with the field of crystal plasticity the group will at first aim at developing, optimizing, and accelerating appropriate numerical and homogenization schemes to lead the field of computational mechanics of polycrystals to rapid industrial maturity.

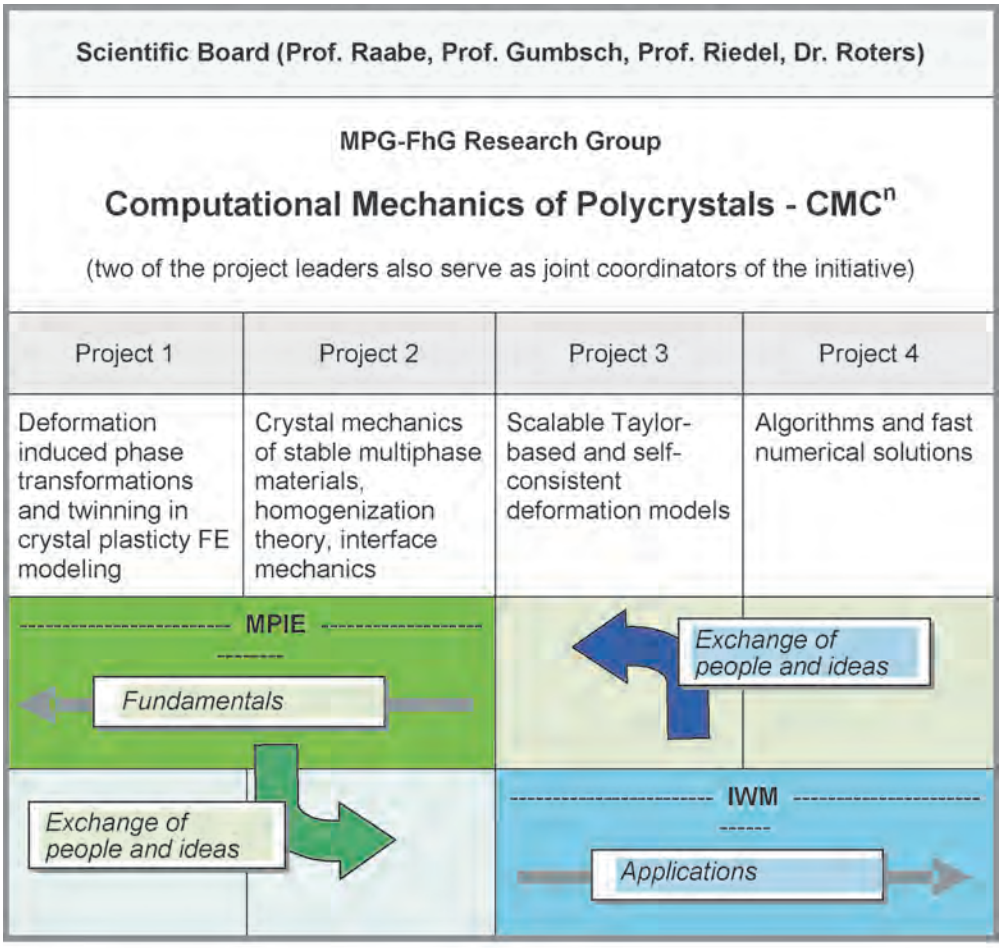
These two aspects, i.e. the micromechanical and metallurgical fundamentals and the engineering optimization of computational polycrystal mechanics methods is an ideal domain for the close cooperation between the Max Planck Society and Fraunhofer Society in the form of the first joint research group between these two societies promoting the label “Engineering Made in Germany“.



Top: Orientation image obtained from an EBSD experiment (inverse pole figure color code) illustrating the crystallography of the grain structure including annealing twins in a X5Mn25Al3Si3 TWIP-steel.

Bottom: Micrograph pertaining to the orientation image above indicating traces of localized deformation, i.e. twinning or slip. The deformation corresponds to planes of maximum Schmid factor (after 1% global strain). Courtesy S. Kobayashi.

The different aspects outlined above are split into four project branches of the initiative (two located in Düsseldorf and two in Freiburg) as shown in the organization chart below. Within the first branch (MPI Düsseldorf) the deformation kinetics usually implemented into constitutive formulations for anisotropic mechanics are to be extended by considering mechanical twinning and transformation of metastable phases in addition to dislocation slip. Both mechanisms contribute significantly to plastic deformation in modern alloys, e.g. lightweight Mg-base materials, TWIP (twinning induced plasticity), and TRIP (transformation induced plasticity) steels. In order to formulate the respective models, corresponding electron microscopy experiments are performed to unveil important details such as associated with the nucleation of deformation twins and their morphology during deformation-induced expansion. The second project branch (MPI Düsseldorf) deals with predicting the plastic response of (meta)stable multiphase materials. Hence, a more detailed knowledge of the microscopic load sharing mechanisms among the different phases during deformation under various types of macroscopic loading boundary conditions is essential. This non-trivial problem can be tackled by assuming different coarse-graining schemes, e.g. isostrain or self-consistent approaches such as pursued in the third project branch (IWM Freiburg), or by extending the simulation scale into the microscopic range. The then necessary understanding of interface mechanics would additionally open up possibilities to capture important aspects of fracture initiation. The different constitutive and numerical modeling challenges outlined above are as a rule computationally more demanding than the requirements typically encountered in the case of the isotropic or yield surface plasticity laws which are presently employed. In order to keep such novel and more complex constitutive laws tractable at an industrial scale the last project branch (IWM Freiburg) is focused on efficient implementation and optimization schemes.



***MPIE**: Max-Planck-Institut für Eisenforschung, Düsseldorf*

***IWM**: Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg*

Aachen Institute for Advanced Study in Computational Engineering Science (AICES)

Marek Behr [+)] *, Dierk Raabe* [#)]

[+)] RWTH Aachen University, [#)] Max-Planck-Institut für Eisenforschung

Introduction. In Fall 2006, the Graduate School Aachen Institute for Advanced Study in Computational Engineering Science (AICES) has been established within the framework of the Excellence Initiative of the German federal and state governments. The Max-Planck-Institut für Eisenforschung is, together with the Research Centre Jülich, the leading academic partner of RWTH Aachen in this initiative.

AICES is designed to provide education to a new generation of graduates, who will receive thorough training at the interface of classical engineering, materials science, applied mathematics and computer science. With its interdisciplinary and method-oriented focus, AICES stays abreast of the fast-paced developments within the comparatively young discipline of simulation-based engineering science, which will decisively shape the future technological development. In this way, AICES ultimately addresses the socioeconomic demands for innovative scientific discovery processes and industrial research and development processes.

AICES will focus on unique and challenging aspects of computational design and analysis, such as multiscale problems, where length scales the size of a molecule or cell interact with much larger scales at which engineered systems are being developed. The Graduate School complements and strengthens the activities already existing at RWTH Aachen and at the Max Planck Institut für Eisenforschung.

AICES is spearheaded by 14 RWTH institutes and the Max-Planck-Institut für Eisenforschung. Approximately 100 doctoral candidates from all partner institutes will participate in the structured research and training programme. By means of an improved student/teacher ratio, among others, it will be ensured that the students are being supported more intensively, which will lead to a reduction of the duration of studies and, at the same time, to a higher qualification of the graduates. In addition, 20 highly-talented candidates will be testing the waters in an intensive fast-track method-oriented curriculum, thus contributing to a shortening of the nominal duration of academic training in Germany. Other innovative elements of AICES include a regional outreach component and seed funds for experimental/computational collaborations.

Academic Aims. Computational engineering already plays a central role in process and product design, production planning, and operations, while computational science has joined the analytical and experimental avenues of investigation as a widely-accepted third pillar of scientific inquiry. The following development trends are currently apparent: an increasing intricacy of the physical or engineering systems being analyzed (complexity), a growing range of interacting scales which must be considered at once (multiscale), larger numbers of interacting physical phenomena that are inseparable (multiphysics), and, demands for best-design identification with reduced input from human intuition (optimization). To address these challenges, the graduate school sets out to advance the computational engineering science in three critical areas of *synthesis*: model identification and discovery supported by model-based experimentation (MEXA), (ii) understanding scale interaction and scale integration, and optimal design and operation of engineered systems, including both the products as well as manufacturing processes. These diverse objectives share a common trait, in that they are examples of *broadly-defined inverse problems*. Such problems are conceptually different from *direct analysis problems* that have been the cornerstone of science and engineering for centuries. In direct computational analysis problems, the system output is determined as a result of given system characteristics and inputs, in direct analogy to an experimental analysis. In inverse problems on the other hand, system inputs, system parameters, or any other internal characteristics of the system are determined on the basis of observations and measurements of outputs of a real system or of the given specifications of an engineered system with desired properties. In model identification problems, either some characteristics of (at least) one of the models, or model interaction mechanism, are yet to be determined, and the computational analysis is performed repeatedly while the results are compared against either experimental data, or computational results obtained with a more fundamental (and presumably more compute-intensive) model. In systems design problems, other aspects of the system are sought, e.g., network structure, geometrical shape or time-varying control profiles, and the computations

are iteratively repeated while comparing the results against some measure of system performance. It is important to note that, while direct problems can be addressed *with* or *without* modelling and computation by mere experimentation and measurement, models and computational methods are a crucial element of inverse problems, as they, loosely speaking, connect measured output data to input data or systems characteristics that cannot be accessed directly in the course of the experiments.

The specific areas of expertise of the principal investigators form the initial group of AICES research topics. Three categories are mainly taken into account, namely, (1) applications and models from the fields of materials and chemical engineering, transportation, electrical engineering, life sciences and geo sciences; (2) mathematical and numerical methods such as in the field of discretization and optimization; and (3) computational tools and infrastructure.

Christian Doppler Laboratory for Polymer / Metal Interfaces

G. Grundmeier, N. Fink, G. Klimow, V. Popova, R. Vlasak, M. Valtiner, P. Lehtinen

The Christian Doppler Laboratory for Polymer/Metal Interfaces funded by the Christian Doppler Society in Austria was established at the MPI für Eisenforschung in April 2003. Dr. Guido Grundmeier is leading this laboratory, which cooperates with voestalpine Stahl Linz and Henkel Austria as industrial partners. Currently, six scientific co-workers are working in the frame of three research modules.

The primary goal of the Christian Doppler Laboratory for Polymer/Metal Interfaces is to understand fundamental mechanisms of adhesion and de-adhesion at modified polymer/metal interfaces and to develop concepts for advanced interface design based on the gained mechanistic understanding.

Current research modules focus on the analysis of principle mechanisms of de-adhesion processes of coatings from galvanised steel in certain cases:

- Delamination starting from a defect down to zinc
- De-adhesion under mechanical load at high water activities
- Delamination from cut-edges

In addition, a fundamental understanding of the function of new environmentally friendly thin conversion layers and their influence on the stability of interfaces is underway as in the near future these new layers will widely replace the established methods of metal pre-treatment.

Methods of electrochemical, spectroscopic and microscopic analysis are further developed to enable the characterisation of processes like film formation on heterogeneous metal surfaces or degradation of interfaces. Scanning Kelvin Probe (SKP - detection of potential changes due to corrosion processes), Infrared Reflection Absorption Spectroscopy (IRRAS - detection of changes in surface chemistry) and Surface-Enhanced Infrared Absorption (SEIRA - analysis of water at the polymer/metal interface) are adapted to the respective scientific questions. These techniques allow the analysis of ultra thin layers and buried interfaces even under corrosive conditions. Complementary investigations are dedicated to the molecular understanding of adhesion based on the application of Chemical Force Microscopy and Single Molecule Adhesion Studies. These studies are combined with quantum mechanical simulations.

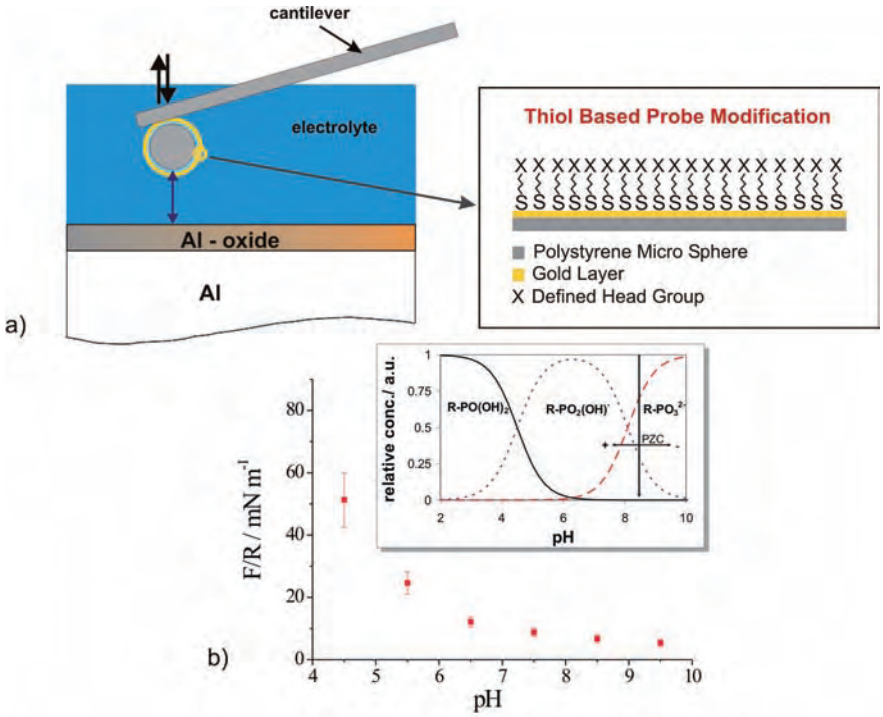


Fig. 1: *(a) Experimental set-up of the Force-Distance analysis under pH control and structure of the surface of the Thiol based modified probe. (b) Results of force distance measurements at different pH values for phosphonate as defined head group of the probe .*

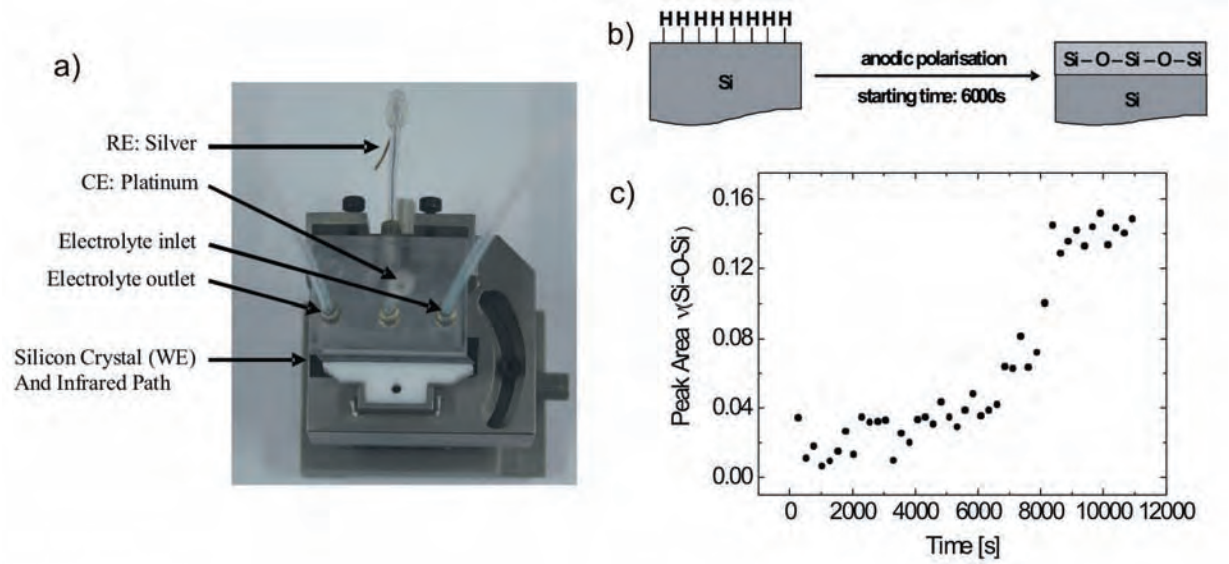


Fig. 2: *(a) The new experimental setup for in situ ATR-FTIR and Electrochemical Impedance Spectroscopy (EIS) analysis, (b) schematic of the Si-O formation on H-terminated Si surface and (c) evaluation of the Si-O peak area (FTIR) after anodic polarisation (t=6000s).*

Research module 1: A new high resolution AFM (JPK, Nanowizard) allows the measurement of force distance curves which are performed under pH control. This pH control allows the modification both of the surface state of the Al substrate and of the state of protonation of the head group of the chemical modified sphere glued to a tipless AFM cantilever (see Fig. 1). One test series is shown in Fig. 1b with a phosphonate group chosen as the terminating chemical group. The decrease of the adhesion force evaluated from several force distance measurements with increasing pH values gets quite obvious here.

Research module 2: The formation of microscopic defects of thin films on metals is studied by forming experiments. Scanning Electron Microscopy microscopic analysis of the films is combined with EBSD to observe changes in the surface structure and de-adhesion phenomena as a function of the grain orientation of the metal. The combination of the forming apparatus with a capillary cell for electrochemical measurements allows the in situ analysis of electrochemical impedance spectroscopy (EIS) during the forming process. This combination is feasible as a result of the reduction of the analysis time of EIS to 1-2 min for each measurement and allows the evaluation of the formability of different organic layers within 20 minutes. A small chamber around the capillary cell also allows electrochemical investigations during the forming process in the absence of oxygen.

In addition, Scanning Kelvin Probe (SKP) measurements of galvanised steel samples covered with a thin conversion layer and a model lacquer as top coat are performed to analyse both the mobility of hydrated ions and the delamination kinetics compared to a non modified sample. The results show a strong inhibition both of the mobility of hydrated ions and of the electrochemical delamination process in the presence of a conversion layer. Supplementary analysis of electrochemical current-potential curves and impedance measurements emphasise the inhibiting character of the conversion films deposited on galvanised steel sample.

Research module 3: The use of SEIRA-Attenuated Total Reflection (SEIRA-ATR) allows the study of water up-take at the interface of thin films and the underlying substrate to be determined, thus revealing the kinetics of wet de-adhesion to be correlated to the water activity. In addition, Infrared Reflection Absorption Spectroscopy and localised electrochemical analyses (impedance measurements at the interface) were recently combined based on a new experimental setup (see Fig. 2). The sensitivity to analyse layers in sub-nanometer scale was proven by the measurement of the oxidation of H-terminated Si surfaces (Fig. 2c).

A similar experimental setup was developed for the use of larger substrates. This new setup was successful for the analysis of the water uptake of epoxy/amine adhesives. The resulting diffusion coefficients gained from both FTIR-ATR and EIS measurements were in excellent agreement.

High Resolution 2D and 3D Orientation Microscopy in SEM and TEM

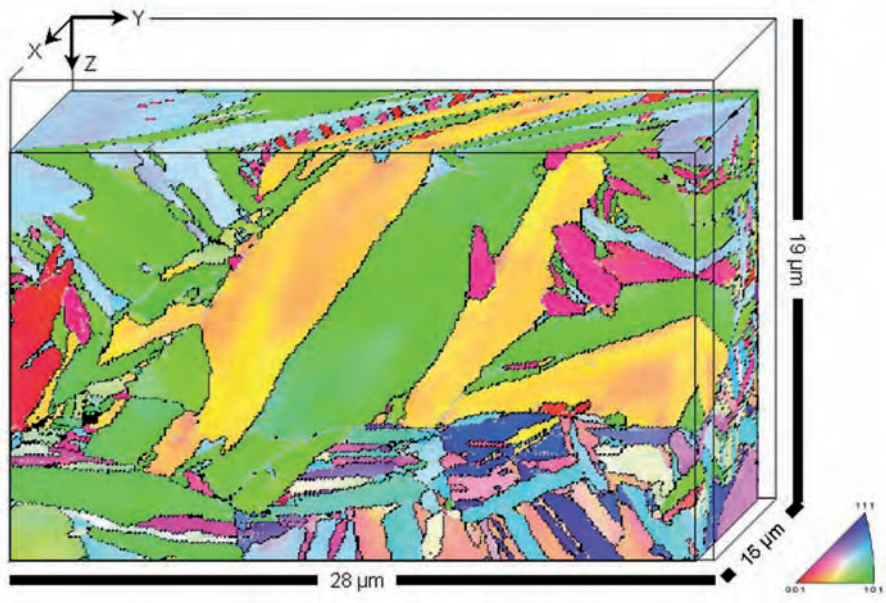
S. Zaefferer

The term orientation microscopy (ORM) comprises a number of techniques which are based on the spatially resolved measurement of crystallographic phases and orientations and the subsequent reconstruction of microstructures and textures from these data. These techniques allow to perform materialography on a new, fully quantitative level in terms of stereology (e.g. size, shape, number and arrangement of grains and phases) and crystallography (e.g. characterisation of interfaces, texture, phases, orientation gradients).

The currently most popular ORM methods are those based on electron diffraction in electron microscopes. In the scanning electron microscope (SEM) the electron backscatter diffraction (EBSD) technique is the most powerful method. It is based on the fully automated analysis of EBSD patterns. With the field emission gun SEM available at MPIE (JEOL JSM 6500 F with EDAX/TSL EBSD system) a spatial resolution of EBSD-based orientation microscopy in the order of 20 to 50 nm, depending on the material, is obtained. Acquisition speed reaches currently almost 80 patterns per second, meaning that maps with several 100.000 points can be measured in about 1 to 2 h.

The EBSD technique recently expands into two new directions: first, in-situ heating and deformation experiments are made possible by a dedicated heating and straining stage for the SEM. The heating stage allows EBSD-observation of processes up to about 850°C which is high enough to follow, for example, the intercritical annealing process in TRIP steels. In-situ straining (compression, tension, shearing) experiments furthermore allow to follow the formation of deformation patterns, twins or martensite, and the occurrence of crystal rotations.

Second, 3-dimensional orientation microscopy is now made possible by the combination of EBSD-based ORM with serial sectioning in a FIB (focused ion beam)-SEM. 3D ORM enables the full characterisation of interfaces (i.e. grain and phase boundaries) and the correct determination of all volume-oriented stereologic values. The system at MPIE is installed on a Zeiss 1540 XB instrument equipped with a TSL/EDAX EBSD system. The software that allows the fully automated serial sectioning and EBSD map acquisition has been written in house in collaboration with EDAX/TSL and Zeiss. Currently a volume-pixel resolution of 100 x 100 x 100 nm³ is reached as a standard but 50 x 50 x 50 nm³ will be achieved in the near future. As an example the figure shows the 3D microstructure of martensite in an Fe-28-Ni alloy (the sample has been obtained from Prof. N. Tsuji, Osaka University).



3D microstructure of martensite in an Fe-28-Ni alloy obtained by ORM.

For extremely highly deformed metals or very fine grained material the resolution of EBSD-based ORM is not sufficient. In this case ORM techniques for transmission electron microscopy (TEM) have to be applied. At MPIE various automatic and semi-automatic techniques are installed on a Philips CM 200 TEM. They are based on the evaluation of spot and Kikuchi patterns and allow reaching a spatial resolution of 10 nm. The spot pattern technique can be applied even on highestly deformed materials.

Ultra-High-Vacuum (UHV) Laboratory for in-situ Investigations

M. Rohwerder

Besides standard surface analysis tools the UHV lab provides dedicated UHV based surface preparation and coating facilities. At the centre of the laboratory is a multifunctional UHV system, which combines several surface treatment and preparation units with a number of sophisticated state-of-the-art surface analytical systems. The concept of this complex unit is to enable the transfer of samples between the different units at any user-defined stage of the sample treatment and permits surface analytical characterisation without exposure to air. Thus, complex processes such as plasma treatment or initial stages of oxide film growth can be studied at different stages.

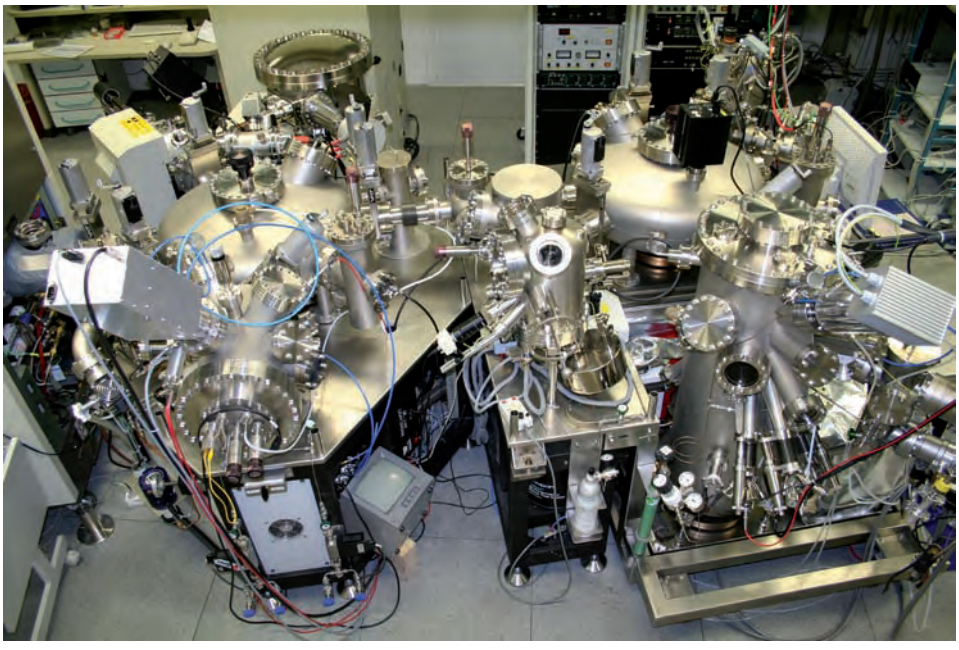
The different units are grouped around two distribution chambers. Attached to the first distribution chamber are the routine surface analytical instruments, the small spot ESCA (PHI Quantum 2000) and the ToF-SIMS (PHI TRIFT II), as well as two process chambers not usually found with UHV systems, i.e., the plasma chamber and the high-temperature oxidation chamber.

A high percentage of the samples investigated in these instruments is not prepared in the UHV system itself, but comes from external corrosion and delamination experiments. For this reason, the first distribution chamber is referred to as the ***service part***. Within this part of the system, the base pressure may not always stay within the specified pressure range for the distribution chambers (10^{-10} to 10^{-9} mbar).

The second part of the system is referred to as the ***surface physics part***. Here a dedicated preparation chamber, equipped with LEED/AES and an ion gun, an MBE chamber, allowing the well-defined evaporation of model alloys and oxides, and a variable temperature STM (VT-STM, Omicron) are grouped around the second distribution chamber, which is in turn connected to the first one. In this part, mandatory precautions must be followed in order to maintain a base pressure within the 10^{-10} mbar range.

Sample transfer between the different units can be carried out quickly and simply. This is guaranteed by a sophisticated sample transfer and piggy-back concept between the different units. Sample transfer is also possible to a VG Microlab (ESCA and SAM), to the LEO FE-SEM and to a glove-box (allowing electrochemical experiments under controlled conditions - below 1ppm oxygen) via a UHV transfer vessel that can be attached to the system's loading locks.

While most of the specialised systems (such as the VT-STM, LEED or also the MBE) are more or less reserved for special projects and their use is restricted to a limited number of qualified personal, it is an integral part of the lab´s concept to provide measurements with the standard surface analytical equipment, such as the Quantum, the TRIFT or the Microlab, on a routine basis to all interested parties.



Multifunctional ultra-high-vacuum system.

Rapid Solidification Laboratory

J. Gnauk

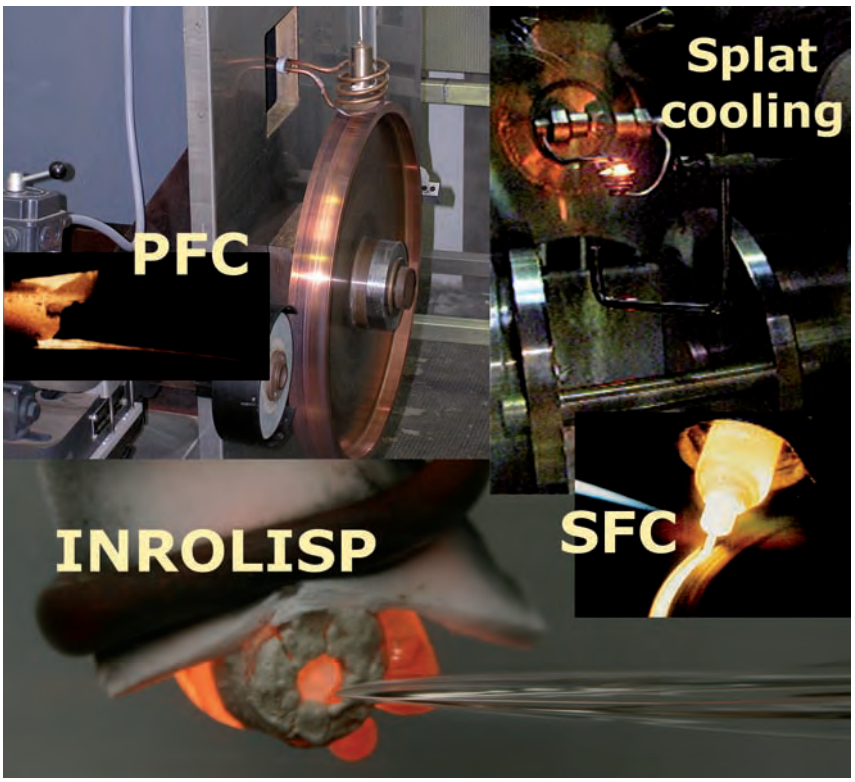
Rapidly solidified materials provide special mechanical attributes like high strength and ductility and special magnetic properties like soft magnetism due to the achieved segregation-free, nano-crystalline or amorphous microstructure, depending on the material and its cooling rate during solidification.

In the rapid solidification laboratory of the MPIE, several facilities for the production of high cooling rates are located. A melt drop furnace and a splat cooling facility, operating with a modified levitation melting unit are used to create rapidly solidified materials with a minimum of technical effort. The facilities enable to examine small amounts of many different compositions, concerning their respective material properties like lattice constants or coercive field strength. Thanks to the levitation melt unit, also high reactive and high temperature materials can be processed.

Larger amounts of material can be produced as ribbons in the planar flow casting facility (PFC), where the liquid melt is cast onto a rotating wheel of copper or steel. Without any active cooling mechanisms, cooling rates of 10^4 K/s can easily be achieved. With extra downstream cooling, also 10^5 K/s is possible. The ribbons are 50 to 150µm in thickness, possessing a width of 5-20mm, depending on the used nozzle.

In contrast to the PFC ribbons, the in-rotating-liquid-spinning (INROLISP) facility produces small wires and fibres with diameters of 40-150µm in a continuous casting process, injecting a small melt jet into a liquid coolant. The cooling rates of 10^4 to 10^5 K/s are similar to the rates of the PFC and depend, besides the casting parameters itself, strongly on the used coolant.

Substituting the coolant basin with a round grooved copper profile, the INROLISP facility can be converted into a shape flow casting (SFC) unit. It can be used for the near netshape casting of wires with diameters ranging from 1 to 3 mm by directly casting the melt into a guiding groove of the horizontally rotating wheel, achieving cooling rates of 10^3 K/s. These cooling rates are comparable with the ones of the twin roll caster, located in the Department of Material Diagnostics and Steel Technology.



Overview of the PFC (planar flow casting), splat cooling, INROLISP (in-rotating-liquid-spinning), and SFC (shape flow casting) facilities for rapid solidification.

High-Performance Computer Cluster

S. Boeck

The *ab initio* atomistic simulation tools developed and applied by the Computational Materials Design department are numerically highly demanding and require high-performance supercomputers. Therefore, one of the first activities of the new department was a price/performance evaluation of various computer platforms and the acquisition of a high performance Opteron computer cluster. The operation of the cluster started in Sept. 2005. Due to the constant high demand in computer power the cluster has been expanded in Nov. 2006.

In the present configuration the cluster contains 320 CPU cores and a total memory of 960 GB RAM. The energy consumption (=heat production) is as large as 60 kW. Conventionally cooled computer centres would require an air-conditioning of a fairly large volume. We have therefore chosen a water-based cooling system that combines various advantages: (a) Only the air volume inside the racks has to be cooled, and thus the energy loss can be kept minimal. The system is fully scalable. (b) Internal fans can cope with the hot spot problem. Hence, even doubled or quadrupled node densities can be accomplished. Auxiliary devices such as switches, power supplies, KVMs are fully scalable to allow an easy extension of the number of nodes. Further, instead of cascading many small network switches only few but high capacity switches interconnect the nodes. This solution ensures a high data throughput between the nodes while reducing costs as well as administrative efforts. (c) The highly packed nodes require minimal space (only 4 racks instead of 6-8).

The computer centre also includes computing services such as file/backup which are crucial for performing simulations as well as method/code development. We combined advanced storage systems (NetApp, Raid level 6, hourly file system snapshots, NFS, CIFS) with conventional storage systems (Raid level 5) to provide a total disk space of 24 TB. To ensure straightforward implementations of future stages of expansion a recent and cross-platform administration tool (scVenus) has been selected. This tool allows platform independent administration and maps user, software, and file space management to the native methods.

In order to offer users an intuitive and transparent handling of the system and to guarantee computational efficiency, newest hardware and software technologies have been combined. For example, the entire (heterogeneous) PC environment of the CM department has been incorporated into the cluster network. Computers are virtually mapped to a huge single system. No login (single-sign in), transfer of files and other daily tedious user jobs have to be done. Furthermore, users can freely choose between Windows and Linux as their PC's host system while accessing the corresponding counterpart by XWin32 or RDesktop. All file spaces (home, raid, san, scratch) are mapped transparently.

High-performance computer cluster with 320 CPU cores, 960 GB Ram, and 24 TB HDD integrated in water-cooled rack systems.

Currently the system consists of 170 clients, the final setup is supposed to included approximately 450-500 clients. In order to reduce the impact of potential hardware failures of these clients to users various control concepts have been merged. First, vital components of the system are monitored every 30 seconds. Even minor problems/faults can be thus promptly identified. Failures of critical components (such as disks of the file servers, redundant power supplies) trigger automatic ordering of spare components via email („self-healing"). Even in case of a broken PC the user can continue working almost without interruption: Our unattended network installation of PCs (cross platform) can reinstall spare PCs within a short time. Since no static methods (such as imaging) are used this approach works even for very different PC architectures. Second, a constantly and automatically monitoring of RAM usage, disk usage, and network traffic allows to quickly identify limitations of the system and to extend the system correspondingly. In conclusion, the concept behind the computer centre is a combination of hard and software fine-tuning to achieve peak computational performance and various methods to provide a user-friendly computer environment.

Central Facilities

Materials Preparation

J. Gnauk

Research and development of new materials and processes require the capability to produce materials according to particular specifications. The institute owns specific facilities to produce and refine materials according to the scientific and technological needs of the research groups within the institute.

Alloy preparation. The two materials related departments of the institute, Materials Technology (Frommeyer) and Material Diagnostics and Steel Technology (Pyzalla) have a variety of sophisticated technical equipments to prepare special alloys as single and polycrystalline samples.

Several ***induction furnaces*** are available to produce different quantities of materials. Small amounts (about 350 to 850 g) of special alloys with melting temperatures up to about 1850 °C are routinely prepared by induction melting in ceramic crucibles in vacuum (2×10^{-5} mbar) or inert gas to obtain cylindrical ingots with 20 to 40 mm in diameter and up to 200 mm in length. For the production of medium amounts of pure metals and alloys (ingots up to 7 kg), two ***vacuum induction furnaces*** with a basic pressure of 10^{-7} mbar are available. Melting of larger amounts of material melts in vacuum or desired atmosphere can be performed in two bigger furnaces, coupled with a facility for pilot test sampling with a maximum capacity of 80 kg and equipped with a 100 kW medium frequency generator. A typical application is the production of iron-based alloys with melting temperatures up to 1800 °C. A ***high pressure induction furnace*** with maximum pressures of 100 bar with a capacity of 10 kg material, operating with a maximum power supply of 50 kW allows to keep melts of earth alkaline, manganese or rare earth metals with higher partial vapour pressure at high temperature in order to prevent vaporisation.

To melt highly reactive materials, two different facilities are available. One is an ***electric arc furnace*** with 300 g capacity, equipped with a tilting mould. In addition to this, an ***induction levitation melting unit*** is used for the preparation of small amounts (350 g maximum) of polycrystalline high-purity alloys exhibiting high oxygen, nitrogen or hydrogen affinity. Melting temperatures up to about 1900 °C are achieved, and for subsequent solidification cold copper moulds are installed in a vacuum or inert gas chamber. Some ***Tammann furnaces*** (electrical resistance carbon furnaces) with maximum operation temperature of 3000 °C enable to process nonmetallic, non-inductive coupling materials under inert gas atmosphere.

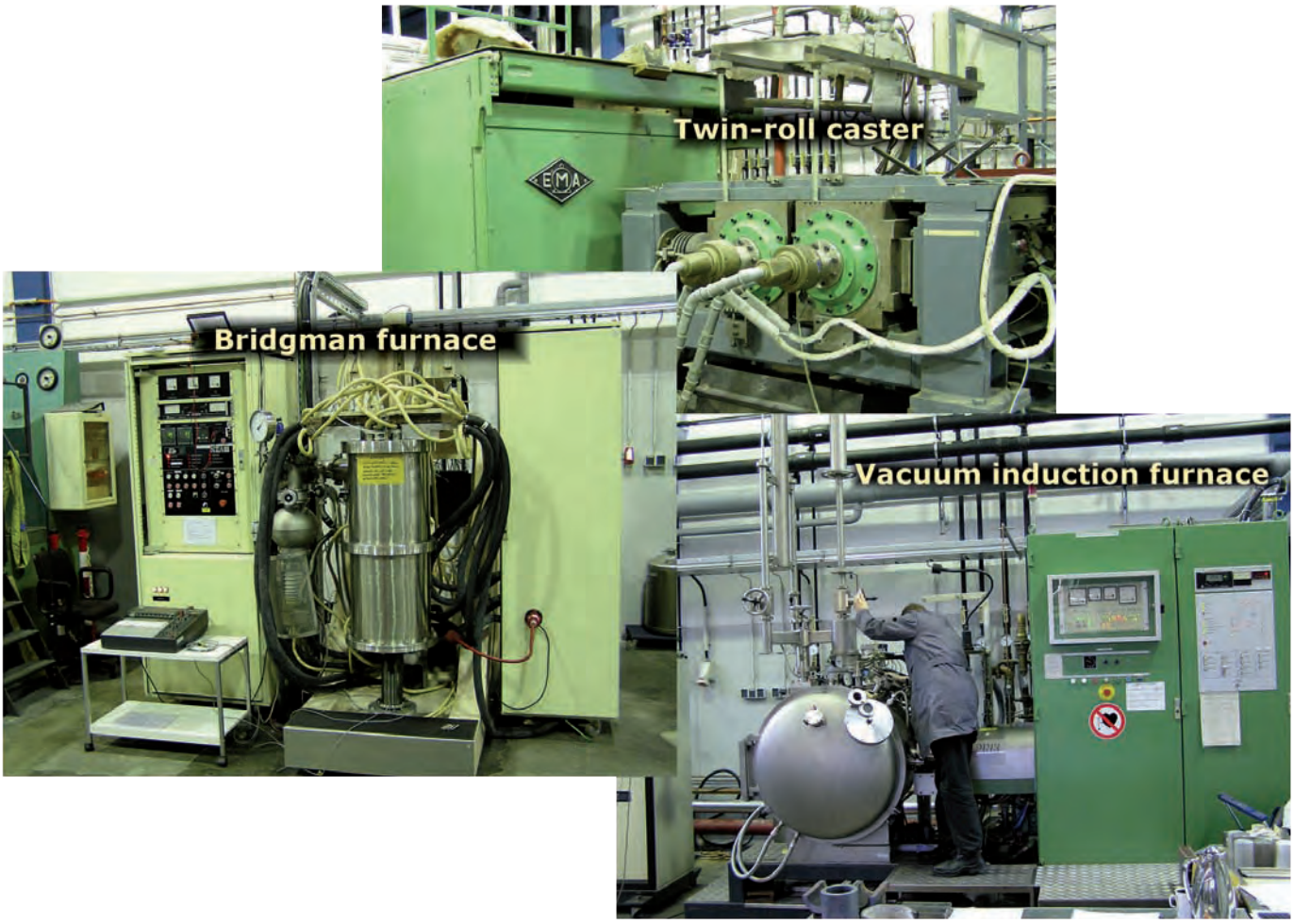
Specific solidification techniques. Single crystals with up to 40 mm in diameter and 130 mm in length of diverse alloys with melting temperatures up to 2000 °C can be prepared in ceramic crucibles in vacuum or inert gas atmosphere using a modified ***Bridgman technique***. Two facilities are available, one with the additional possibility to apply pressures of up to ten bar during the process.

Single crystal growth and high purification of metals using the method of zone refining can be performed by a 75 kW ***electron beam melting furnace***. The molten zone is produced by a circular cathode of tungsten, which is moved vertically along the sample.

In addition to the Bridgman type furnaces, which are specifically designed for controlled slow cooling processes, two units for rapidly solidified materials are also available. These are a ***melt drop furnace*** and a ***splat cooling facility***, operating with a modified levitation melting unit.

Near net shape casting. Two ***thin strip casters*** for direct strip casting related to Bessemer's process are operating in the Department of Material Diagnostics and Steel Technology. The as-cast materials may be peritectic or other low carbon steels as well as stainless steels and non-ferrous metals. One caster is equipped with a 150 kW induction furnace with a maximum crucible capacity of 200 kg. The produced steel strips have a thickness of 1 to 4 mm and a strip width of 120 mm. The second caster is a slightly smaller facility (30 kW furnace, maximum capacity 10 kg, strip width of 65 mm). It has the unique feature of a full housing of the caster and of the strip casting process, i.e. the process can be carried out in an inert gas atmosphere.

The institute is also equipped with several facilities for rapid solidification as a ***shape flow casting*** (SFC) and a ***planar flow casting*** (PFC) facility for



Examples of materials preparation facilities at the MPIE.

the fabrication of metallic fibres, wires and ribbons or foils. These outstanding facilities are described on p.25 in the section on 'Outstanding Scientific Laboratories'.

Thermal treatment. In addition to the casting facilities mentioned above, several annealing furnaces are available to manipulate the microstructure and phase distribution after the casting process. For the heat treatment several annealing furnaces in various geometries and dimensions with temperatures up to 1700 °C are present, partially with protective atmosphere or vacuum.

Mechanical alloying. Powder metallurgical processing like mechanical alloying can be carried out using a planetary ball mill, partially filled with hard and heat resistant steel or cemented carbide balls (5 to 11 mm in diameter) and a capacity of 500 ml in an inert gas atmosphere. Another high energy ball mill (attritor) with a total capacity of 8 litres serves for the production of larger amounts of material. To form billets of metal powder, isostatic pressing with pressures up to 3500 bar can be performed with a cold isostatic press possessing a cylindrical chamber of 400 mm in length and 200 mm in diameter.

Metallography

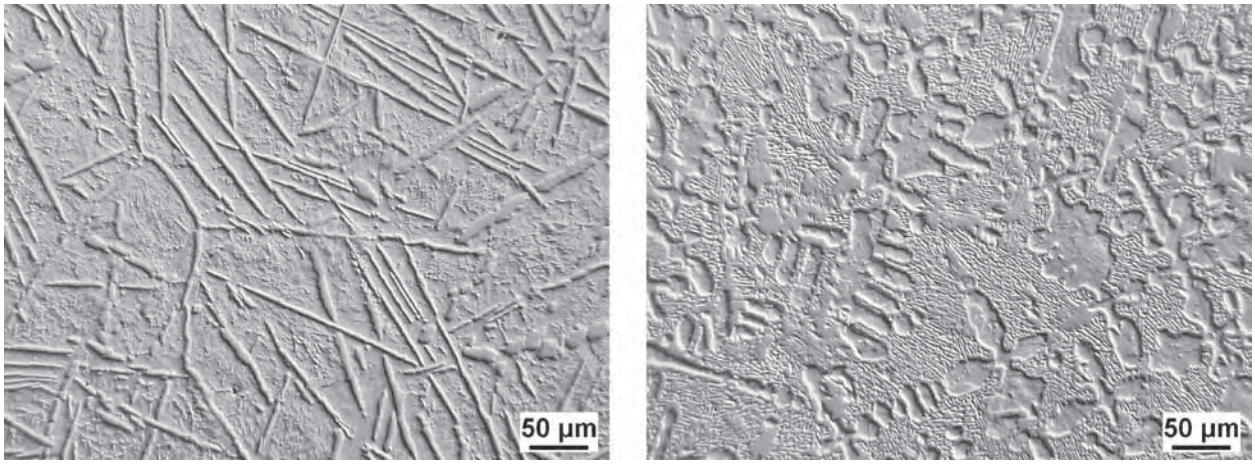
S. Zaefferer

Task of the service group Metallography is to perform metallographic work for the different groups of the institute or to instruct and support the members of the groups (for example PhD students and postdocs) with these tasks. Currently the group consists of 5 experienced metallographic assistants. The services offered by the group include the metallographic preparation of metallic, intermetallic and non-metallic samples for different observation techniques or for further processing and the observation and documentation of samples by optical and scanning electron microscopy.

For preparation a large variety of different techniques are available. These include cutting with various techniques, sample mounting (hot and cold, conductive or non-conductive resin, resin-free sample mounting), grinding and various polishing techniques with a wide range of different polishing solutions. Also available is electrolytic polishing. After polishing, samples may be chemically or electrochemically etched to develop the microstructure for further observation. For these tasks a variety of different recipes, with focus on the preparation of microstructures of steels and intermetallics are available. Finally, specimens can be coated by sputtering of gold, iron, copper or carbon.

For the observation of microstructures by optical microscopy various instruments by Leica (Aristomet), Zeiss (Axiomat) and others are available. A wide variety of observation techniques including bright field, dark field, differential interference contrast, polarized light microscopy and macro photography with perpendicular illumination can be applied. Furthermore a hot stage microscope for observation at high temperatures and a micro hardness tester are provided. Photos are either acquired conventionally on photographic film or by high resolution CCD cameras. Digital images are automatically sorted into a digital data base and can be analyzed by software for digital quantitative metallography. An example is displayed in the figure below which shows the microstructure of two different Fe-C alloys that have been enriched with aluminium by a pack-cementation diffusion process.

For observation at higher resolutions a scanning electron microscope Camscan CS4, equipped with an EDX system with a detector with ultra thin window for light element analysis is used. The instrument is run and maintained full time by one of the group members.



Differential interference contrast image of two Fe-C alloys (left Fe1.5 % C, right Fe 3.5 % C) enriched with aluminum in a pack cementation process at 600°C for 24 h. Courtesy of M. Spiegel.

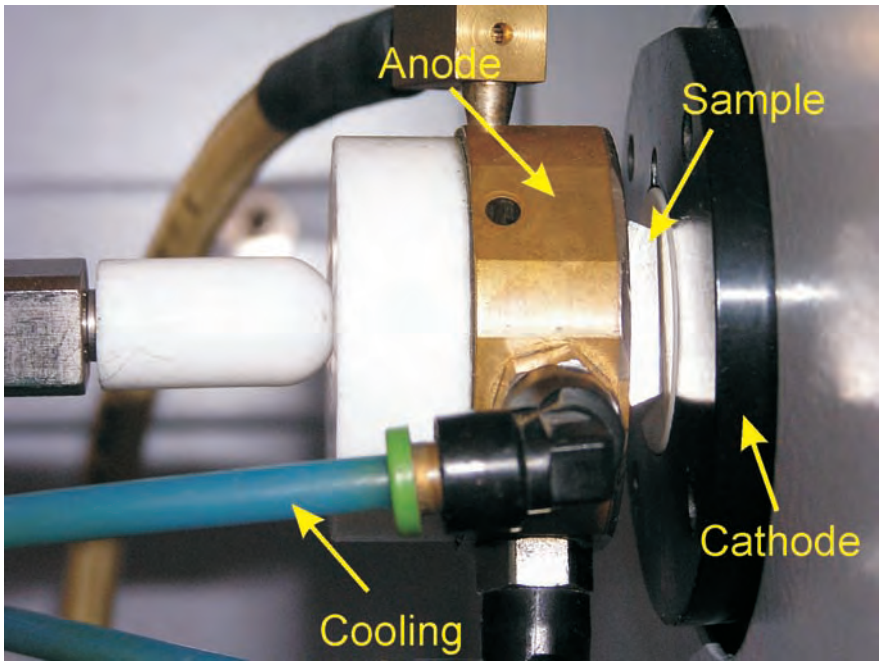
Chemical Analysis

D. Kurz

The knowledge of the chemical composition is an important requirement for the use of materials in chemical experiments and for the characterization of materials. Simultaneous atomic emission spectrometry with inductively coupled plasma and dual view optics (ICP-OES), atomic absorption spectrometry with a flame, graphite furnace and hydride technique (FAAS, ETAAS, CVAAS), ion chromatography (IC), thermal conductivity and infrared absorption are the standard methods used by the group for the analysis of nearly 60 elements in different materials and matrices.

Since January 2006 a new analytical technique is available, a Glow Discharge Optical Emission Spectrometer (GD-OES). This method is very useful to quantify the chemical compositions and the thickness of layers from coated materials. Also it is possible to analyse the interface between the layer and the bulk material as well as the diffusion zone.

During the analysis, a plasma is generated in the analysis chamber by the applied voltage between the anode and the cathode (the sample) in the presence of high purity argon under low pressure. Ionised argon atoms cause sputtering of the sample surface and the sputtered atoms are excited in the plasma to emit light of characteristic wavelengths. There are more than 40 photomultipliers installed for the simultaneous detection of the emitted photons.



Glow discharge optical emission spectrometer (GD-OES).

Computer Network Centre

R. McCormack

The service-oriented Computer Network Centre offers a campus wide high speed „local area network“ (LAN) consisting of over 1500 fast Ethernet ports and nearly 500 gigabit ports in traditional RJ45 copper cabling systems as well as fibre optics ports. The Network Centre also develops, implements and maintains security systems, VPN access, intrusion detection appliances, firewalls and spam gateways as centralised services for approximately 280 users.

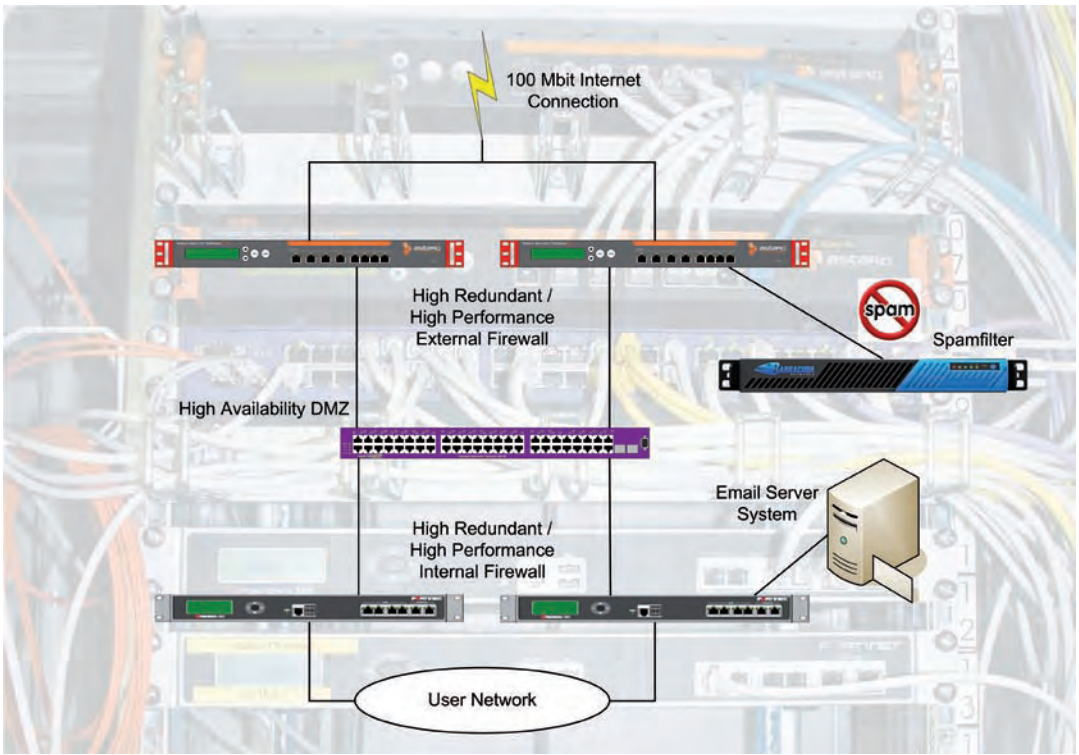
In the last few months the Network Centre has restructured the Internet access technology, security systems and mail infrastructure, which authenticates users against a central Active Directory System.

The Internet access was upgraded from a 34 MBit E3 serial connection to 100 MBit Ethernet making it easier to manage. Due to the cheaper Ethernet hardware, the new access technology is more cost effective than the old system.

The high availability firewall scenario is built up from two identical firewalls on the outside perimeter and two identical firewalls from a different manufacturer on the inside perimeter. Each firewall group is set up to run as a combined high available system. If one firewall suffers a hardware defect, the other system automatically takes over.

The different firewall systems on the outside and inside perimeters are intended to make life difficult for internet culprits due to the fact that a potential security flaw on one firewall system is probably not exploitable on a different firewall system, making this scenario failsafe in more than one way.

The new mail architecture consists of a spam mail gateway and a mail server. All mails arriving from the outside world are systematically scanned for fake senders, invalid recipients and certain keywords. The remaining mails are then scanned for viruses, phishing attempts and checked against a personal user database were each user can block or allow certain bulk emails such as newsletters etc. Currently the system filters out approximately 4800 – 6500 junk emails each day, another 300 are placed in a personal user quarantine which is then forwarded to the user in a daily digest email allowing the user to select certain mails and then decide what to do with them. Mails that pass through the spam gateway then are forwarded to a mail system that runs all mails through another virus check and delivers them to the user mailboxes. The users then can check for mail via Web or WAP, push mail services with Windows CE devices or traditional mail clients. Each user can apply for up to 3 GByte of storage.



Firewall system at the MPIE.

Electronics Workshop

B. Schönberger

The experimental research character of the institute requires a wide range of laboratory equipment, which has to be designed, built and tested by the electronics workgroup in close cooperation with the scientific staff. By combining commercially available devices for process control, data acquisition and data analysis, most research demands can be satisfied. However, it is of particular importance to respond to special research requirements with unique prototype design for low-level measurements, special sensory and high-quality process instrumentation. In recent years, the electronics workgroup has developed exceptional experimental instrumentation, which is considered unique.

An example for this task is the program for controlling a set up for thermo-cyclic investigations with simultaneous data acquisition. All the components, including an infra red radiation furnace with a temperature controller, valve controllers and a gas mixing apparatus with mass flow controllers, are remotely accessed and controlled via serial ports using device specific protocols.

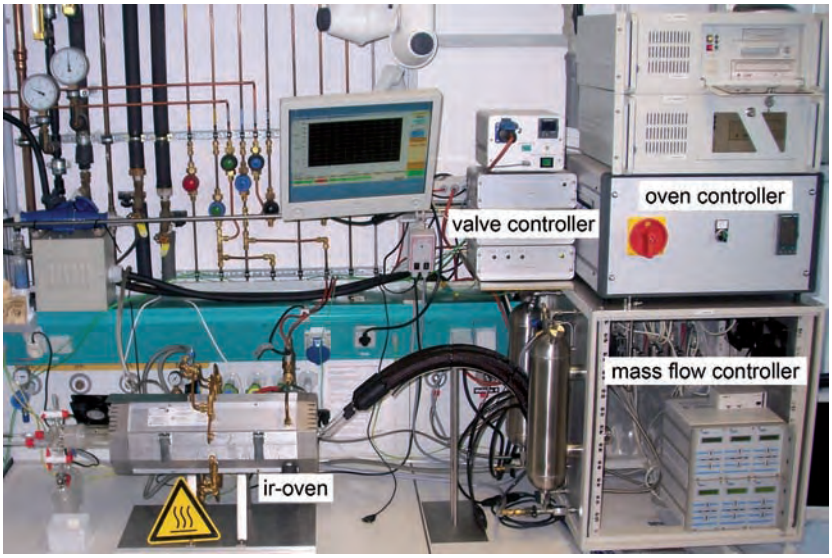
The particular advantage of this program is the fact that it accesses and controls different components made by various manufacturers. The set up shall be used to perform thermo-cyclic experiments with programmable ramps and holding times as well as user-defined arbitrary gas mixtures. Additionally, valves for air-cooling will be controlled.

In order to achieve this, the control program was equipped with a scripting language which uses simple „words“ (set, time, wait, loop, valve…) to access specific functions. The scripted instructions are saved in a text-file. Another file is saved containing information about the desired gas amounts and mixtures as well as the control ranges of the mass flow controllers. These text files can be created and edited with any text editor and subsequently be loaded into the control software, depending on the desired task.

Following a syntax check the designated experimental procedure is visualized on the screen before the experiment is started. For trouble shooting purposes and functional testing of individual components, these can be manually addressed with commands from the user interface. After starting the experiment all readings are recorded and can subsequently be loaded into e.g. Excel files for evaluation of the data. For real time observation of the experimental procedure the given and desired temperatures are shown as graphs next to the numerical displays of the gas concentrations. The correct operation of the mass flow controllers is displayed using color coded fields.

Finally the experimental progress is displayed by giving the active scripted command, the loop count and the total experiment time – this allows a quick and convenient way to control the experiments execution.

Another current project is focused on the process instrumentation of planar flow casting set up. In this case a scanning quotient pyrometer is being developed in order to determine the temperature profiles in the experiment.



Experimental set-up for thermo-cyclic experiments.

Technical Services

M. Winkler

The technical services are divided into multiple sections: technical equipment and installation including the electrical services next to the mechanical workshop. The technical services are responsible for the supply and maintenance of basic services and therefore ensure a failure-free operation of the scientific research performed at the institute. By utilizing a well organized facility-management, which includes routine maintenance and repairs, technical failures can be avoided, providing an ideal environment for scientific progress.

An important issue for the technical services in 2005 / 2006 was the commissioning of the halls 8 and 9, including the office areas. The completion of hall 9 will take place soon, so that it can be handed over to the department WS. The halls – with their outline of 68.72 by 39.20 meters and a height of 11.60 meters will be completely redeveloped and consigned to the institute.

The technical facilities now correspond to the state of the art for modern laboratories and office buildings. They therefore offer the best circumstances for high-end research. The configuration of each new laboratory was realized according to the various requirements of the different departments. Additionally, the laboratories were fitted with cooling-water systems, water supplies, fume hoods, and sub construction fume extraction as well as central gas and pressurized-air supplies. A cooling circuit with 20/30 °C was set up for equipment that is used for experiments and process simulations. This circuit is run by the existing cooling machinery in hall 4, supported by a new free-standing cooler with a rating of 290 kW which was installed on the roof of hall 8. A total of 660 m of piping (DN 25 – DN 100 PE-HD) was installed to ensure the cooling of hall 8.

All installations are controlled from the facility management's primary control unit – this is where all data are processed. The primary control unit is the basis for all controlling and management functions as well as the centralized operation and monitoring of the facility's installations. At present there are a total of 2900 data points using DDC-technology (digital data control) connected to the primary control unit for the entire institute, allowing an effective monitoring of e.g. the air-conditioning systems – 89 of these data points need to be managed in hall 8 alone.

Supplying electrical power to the halls is achieved by installing a new low-voltage unit which is capable of handling loads of up to 2500 amperes. The in feed is handled by two 630 kVA 10kV/400V/230V dry transformers. In total approx. 25,000 m of cabling were installed into hall 8 as well as 12 power distributors.

Renovated hall 8 showing facilities for thermomechanical treatment and metal forming; the large device in the foreground is the WUMSI (Warmumformsimulator, hot working simulator) (Photo: O. Schoplick, Düsseldorf).

In order to guarantee modern data systems technology and telecommunications 10,400 m of fiber optic cabling were installed next to 12,500 m of Cat 7 ethernet cabling and 171 fiber optic connector sockets.

Fire prevention technology was realized using 4,775 m of cabling and 203 smoke detectors (O 400) operating in double line dependency mode. The high ceilings of the halls were fitted with 14 linear smoke detectors, Firerays, equipped with laser technology. All smoke detectors are integrated into the new fire-registering-system. The air-conditioning system has

been fitted with fire shutters which are connected to the facility management's primary control unit using the DDC-bus system.

The handling of heavy objects in the halls is now allowed for by the two new in-door cranes that can each handle 5 tons. The building was adapted to the present thermal containment guidelines. All in all the halls have now been adapted to state-of-the-art technology.

Another noteworthy innovation was the computer cluster with 120 nodes and a cooling power of 60 kW in hall 2, which was installed for the newly established Department of Computational Materials Design.

Mechanical Workshop

R. Selbach

The workshop includes the design engineering office, the actual mechanical workshop including the apprenticeship workshop, the locksmith's shop and the precision mechanics.

Projects and devices are developed and manufactured in close cooperation with scientists and electronics engineers. A wide variety of tasks has to be handled including, e.g., precision mechanics engineering, the construction of devices for special purposes and lightweight constructions.

For design and development, it is standard practice to apply 2D and recently also 3D-CAD software tools.

Apart from the production of round and flat specimens for tensile tests and samples for charpy tests and creep experiments from a wide range of materials, several interesting projects were carried out during the last two years. Some highlights of our work include the construction of a special pulling tool for creep experiments, a new in-situ plasma reaction chamber made of stainless steel, the construction of x/y/z manipulators, a noise control chamber and a stainless steel sample cupboard.

In the apprenticeship workshop of the institute, six apprentices were trained to become industrial mechanics. The apprentices in the third training year made already essential contributions to ongoing projects. In addition we had four trainees doing practical courses in the field of metals.

Library

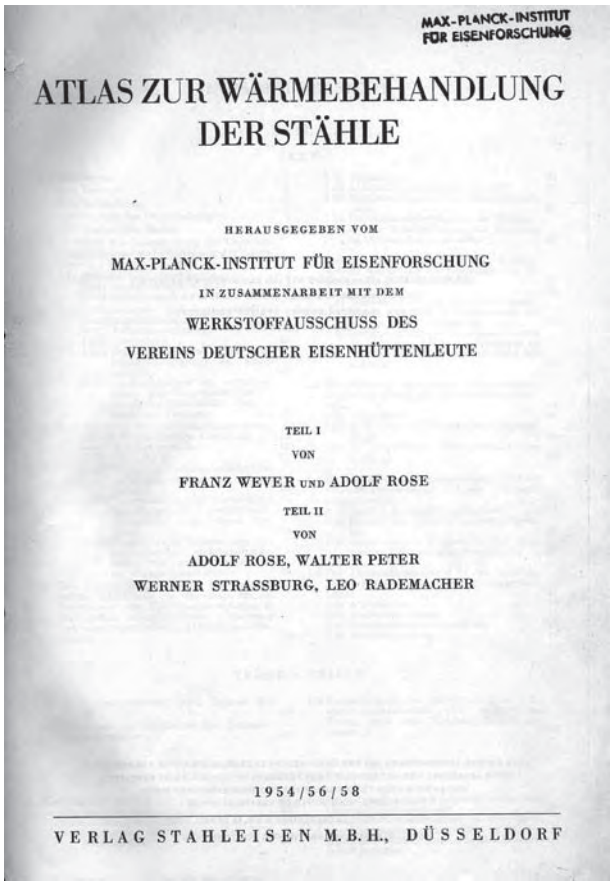
W. Rasp

The institute's library is organized – in contrast to most other public libraries – as a reference library, so that the service function of a lending library is not provided. Unfortunately, there is some restriction to have a direct access to the library because at present it is lodging in a neighbouring building which is part of the Steel Institute VDEh. All together the collection contains nearly 5000 catalogued scientific books. They are grouped into 19 topics, which cover most of the broad range of the institute's scientific interest. Institute employees are allowed to borrow a book temporarily or, with special permission, for a longer term. A searchable database is provided via intranet for all institute co-workers.

Among the basic collection of books, there are a lot of valuable, old volumes as e.g.: Georgius Agricola 'De Re Metallica', Basel 1556; J.K. Kunst und Werckschul/Anderer Theil 'Chymiae ac aliarum Artium Cultore', Nürnberg 1707; Monsieur de Reaumur, de Academie Royale des Sciences, 'L'Art de Convertir le Fer', Paris 1722; Jars Gabriel 'Metallurgische Reisen, I-IV', Berlin 1777-1785. Particularly the well-known book „Atlas zur Wärmebehandlung der Stähle" edited by the Max-Planck-Institut für Eisenforschung in the years 1954 to 1958 should be mentioned, which finds worldwide use in the steel-processing industry, see figure.

Many scientific journals (about 10,000 volumes) are also collected in the library. The oldest of them are 'Zeitschrift für Angewandte Physik' beginning 1848, 'Stahl und Eisen' starting in 1881, 'Zeitschrift für Metallkunde' since 1919 and 'Archiv für das Eisenhüttenwesen' first issued 1927/28 and renamed into 'steel research' in 1985.

These days the number of paper journals in the institute's library is decreasing because of the increasing importance of publications via electronic media. So the institute takes advantage of the Virtual Library (VLib) offered by the Max Planck Society. VLib allows free access to all sort of basic information resources on different electronic platforms by means of the internet. Thus the staff members and guests have a run of about 4300 journals, 1450 of them being licensed for permanent storage by the Max Planck Society. The VLib portal also makes available the library catalogues from 70 different Max Planck Institute libraries as well as those from external libraries. In view of this immense supply of information the institute was able to reduce its own budget for scientific journals considerably.



Cover page of 'Atlas zur Wärmebehandlung der Stähle' edited by Max-Planck-Institut für Eisenforschung. Düsseldorf: Verlag Stahleisen 1954 to 1958.

Administration

H. Wilk

In the end of 2003, preparations to introduce the SAP R3-Software-module „Human Resources“ were concluded. Since January 2004, salaries and wages of the employees are again calculated in the institute and the outsourced computation was discontinued. The new module extends the possibilities to integrate personal data from the personnel division into the accounting system of the institute. External consultants assisted in introducing and customizing this module. The entire information-system SAP R3 will be maintained by the Max Planck Society.

The introduction of another SAP module was concluded too in June 2005. This module integrates cost accounting into the information system and will further refine the already existing possibilities to create statements for revenues and expenditures.

Research contracts funded by third parties are concluded increasingly with industrial partners, besides contracts with public financing. Particularly, agreements on intellectual property rights and their exploitation are object of difficult negotiations. A support agreement with the consulting society Garching Innovation GmbH, Munich, which also carries out the marketing of the know-how of the Max Planck Society, has been signed.

In the last years, many foreign nations were represented at the institute. The large number of foreign employees leads to growing language problems. Especially the fact that research contracts are formulated in increasing number in English is also a special challenge for the administration. Therefore, it was decided to offer the employees English language courses. The first course started in March 2006. Three groups with different level in practice of English language were established. Nearly 25% of employees with unlimited contract take part at the lessons. Before the end of 2006 the board of executives has to decide about continuing these language courses.

In the last two years a new structure for budgetary planning was prepared. It is intended to define a core budget for the institute which takes the necessary financial means needed by the institute into account. Structure and financial requirements of this core budget shall not be negotiated on a yearly basis with the Max Planck Society and the Steel Institute VDEh. Changes in the structure lead to adjustments of the financial means. Special influences (expensive investments, appointments etc.) will not be part of the core budget and these financial requirements have to be negotiated separately. In September 2006 the advisory board of the institute agreed to the planned budget 2007, which is corresponding with these new budgeting guidelines.

PART II.

THE DEPARTMENTS

(in alphabetical order)

Department of Computational Materials Design

J. Neugebauer

Scientific Concept

The mission of the department Computational Materials Design is the description and prediction of material properties by means of computational simulation techniques. With a particular focus on iron and steel, experimental observations shall be understood, relevant physical mechanisms shall be identified and the conditions to obtain a tailored material design shall be predicted.

In order to understand a property on a given length and time scale (being typically the macroscopic scale), it is crucial to understand/simulate the properties and mechanisms on all shorter length and time scales. Due to this hierarchical nature inherent to all materials, multiscale simulation techniques are being developed and applied (Fig. 1). A key expertise of the department is to trace the description back to the atomistic scale, making use of the fundamental laws of quantum theory. A major advantage of this approach is the absence of any empirical or adjustable input parameters. This ensures unbiased simulations with high predictive power and allows for the determination of quantities or properties that are only difficult and/or expensive to measure or not accessible by experiment. These simulation tools therefore nicely complement existing experimental and theoretical tools at the institute and open novel research directions.

The head of the department, Prof. Jörg Neugebauer, and many of the scientific co-workers gained their expertise with developing and applying ab initio based multiscale methods in the field of semiconductor physics, i.e., with materials of high chemical purity and low defect/microstructure density. When the new department at the MPIE was established in May 2005, a first challenge was the transfer of this expertise to metals. Although the ab initio approach is in principle valid independent of the material, the complexity of metallic alloys with respect to chemical composition, their rich phase diagrams and microstructure, and their low chemical purity makes a continuous development and improvement of innovative simulation methods necessary. This

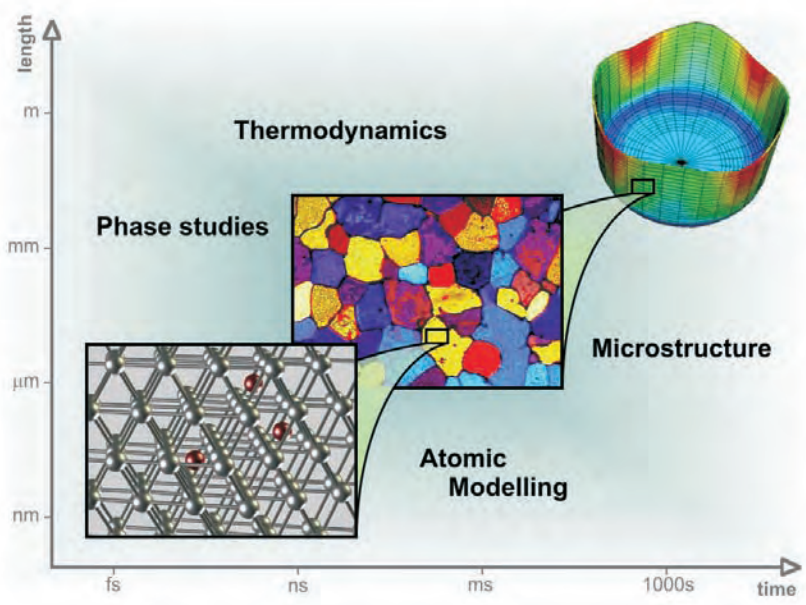


Fig. 1: *Schematic visualization of the hierarchical nature of materials. The properties of a material on the macroscale as relevant e.g. for engineering applications develop over a large range of length and time scales. The aim of the CM department is the development of efficient simulation tools which start at the most fundamental level – the quantum mechanical description of the atomic scale - and extend to all relevant scales.*

is a mission of the entire department. To address the inherent complexity of metallic materials the department consists of research groups which are specialized on various aspects and scales and which develop and apply highly efficient and accurate simulation tools. To address materials issues, which often originate from a collaboration with the other departments of the institute, with industry or other scientific institutions, the expertise of the individual groups is combined.

A major milestone for the department was the procurement and installation of the **Computer Centre** in August 2005 (see page 28). With the availability of the high performance Opteron-Linux cluster the department was able to perform first calculations, benchmarks, code developments etc.

The foundation for an efficient method development is laid in the research group **Algorithm Design and Modelling** headed by S. Boeck. Based on the program packages and visualization tools developed in that group the other scientific groups develop and apply simulation tools covering specialized physical aspects. A major area of method development and research in the department concerns approaches to accurately predict thermodynamic and mechanical properties of materials.

Many properties and processes in materials science, and in particular in steel research, can be directly related to phase diagrams. For this purpose it is important to have a microscopic understanding of all relevant phases and phase transitions for the complete temperature range from the ground state to the melting point. These investigations are performed in the group **Phase studies** headed by T. Hickel. The consideration of thermodynamic effects includes the vibronic and magnetic contributions to the Gibbs free energy. Another important concept to understand temperature dependent effects is related to configurational entropies in complex multi-component alloys. This issue is in the focus of the group **Ab initio thermodynamics,** headed by M. Friak. In order to get a deeper understanding of microstructure formation and evolution, segregation effects and hardening, the group **Microstructure**, headed by L. Lymperakis, develops tools to study first the thermodynamic stability and later also the kinetics of extended defects such as dislocations and grain boundaries.

The studies at the atomic scale in the research groups mentioned above provide an excellent basis to describe a wide range of materials related issues (see e.g. the short papers in part III of this report). However, certain questions such as solidification and heterogeneous nucleation, which are highly relevant for steel casting, are way too complex to be tackled solely by atomistic simulations. It is therefore planned to establish a new research group that is devoted to **Phase Field Simulations.** This group, using parameters calculated by the atomic scale groups, will study various aspects of microstructure formation.

With its wide range of scientific simulation tools the department was quickly able to link to existing research activities within the MPIE as well as to open new areas. For instance, close collaborations with the department of Prof. Raabe, related to mechanical and structural properties of metallic compounds (see p. 125) have been started. There are joint projects with the department of Prof. Stratmann, concerning destruction mechanisms of metals such as hydrogen embrittlement and the delamination of protection layers. The research in the CM department strongly benefits from intensive discussion with members of the department of Prof. Frommeyer about properties in modern light weight/high strength Mn steels. Joint research activities on metallic interfaces together with the department of Prof. Pyzalla will start in 2007.

Since most of the department members had a background in semiconductor physics [1], the department made sure to get in touch with the leading international experts in the field of computational materials design of metals. For example, an international workshop on “Ab initio description of Iron and Steel: Status and future challenges” has been organized and performed at Ringberg Castle in February 2006. Internationally leading experts from different scientific communities (basic research, applied science, industry) presented tutorial-like lectures on their methods and results. In addition, leading scientists in this field came to the MPIE for presentations and intensive discussions, often with all members of the department individually. Vice versa, members of the CM department have been invited to conferences, research institutes and companies to report about the most recent results obtained and the promising applications of ab initio multiscale simulations.

Although the department became operational only in August 2005 with the availability of a high performance computer cluster, the expertise developed by the research groups quickly sparked an interest at various institutions and industrial research labs and was the basis for a number of high-ranking joint research projects which started already or will start in 2007.

Scientific Groups

Algorithm Design and Modeling (S. Boeck)
(since March 2006)

The above mentioned goal of simulating material properties on several time and length scales requires the combination of various methods. The currently existing program packages are mostly designed for certain scales and are difficult to combine, since they are based on incompatible approaches and/or numerical concepts. In order to enable and perform truly multiscale calculations, it is therefore the aim of the group “Algorithm Design and Modeling” to develop a fully flexible and modular approach, which allows incorporating methods of all scales inside the same package.

S/PHI/nX: The group has implemented a new and truly object-oriented library called S/PHI/nX. It is based on a cross platform algebra library developed by the group that is able to map algebraic expressions directly onto high performance numeric library calls (BLAS/LAPACK/FFT). Due to state-of-the-art programming techniques the library combines a user-friendly programming interface reminiscent to Mathematica with peak performance. On top of this algebra library a layer has been developed which provides the algorithms needed to construct an efficient density functional theory (DFT) code. A new hybrid programming technique developed in this group allows a very compact and easy to read implementation of new algorithms (see p. 195). The key is that already the compiler translates expressions written in the Dirac notation into optimized code with peak performance. This approach allowed e.g. an implementation of all algorithms related to the Hamiltonian to be independent of the specific basis. Besides DFT also tight-binding based methods as well as empirical potentials have been implemented to perform large scale simulations.

Specifically for the application of the latter a highly optimized atomic structure library has been developed. Similar to the algebra library also this module automatically maps expressions needed to perform large-scale MD-runs to efficient BLAS/LAPACK function calls. The flexible approach of S/PHI/nX made it easy to implement/test extensions or new algorithms. For example, improved functionals such as the exact exchange formalism have been introduced and successfully applied to study problems which have not been accessible otherwise. An example is the accurate description of bandgaps in widebandgap semiconductors. Another example is the development of fast high-dimensional minimization schemes such as the all-band conjugate gradient algorithm. Currently we focus on the implementation of PAW (Projector Augmented Waves method) in order to speed up the calculations particularly of metallic systems while gaining higher accuracies.

PHInaX: Packages like S/PHI/nX generate huge amounts of data during their calculations. Undoubtedly, interactive 3D visualization is required to comprehend the computed data. Due to the multiscale approach of S/PHI/nX a problem in visualization emerges: Multiscale simulations require multiscale visualization. At the atomic scale DFT describes fairly small atomic structures but creates large data sets containing wave functions as well as various scalar and vector fields. On the other hand employing empirical potentials molecular dynamics runs for systems containing a few million atoms are routinely performed. On the mesoscopic scale one faces huge multidimensional vector and tensor fields, which have to be rendered. Since there is no cross-platform visualization package available, which is able to cope with these requirements, the group has developed a new modular multiscale visualization framework called PHInaX. Since PHInaX is based on the S/PHI/nX libraries the entire functionality and flexibility of S/PHI/nX is reflected in PHInaX. Various new techniques have been introduced that make PHInaX a perfect tool to visualize solids: (a) The underlying periodicity of crystals is implemented directly within the render pipeline. Rendering periodic structures does not require any additional memory or performance compared to visualizing a single supercell. (b) By supporting state-of-the-art graphic card extensions the new tool is able to visualize *interactively* up to 1.000.000 atoms. (c) Diffuse volume rendering based on particle system techniques have been implemented in order to render electronic charge densities and potentials computed from DFT calculations.

Currently the group focuses on two major extensions to PHInaX: First, the setup of a full-featured workbench including job submission and data retrieval and second, an implementation of virtual reality functionality. The aim is the development of a fully integrated platform which allows covering all aspects of a simulation: setting up jobs, job submission, data retrieval, and complete analysis including data visualization as well as a secure data exchange between research groups.

Computational Phase Studies (T. Hickel)
(since September 2005)

The research in the group "Computational Phase Studies" is focussed on the investigation of (meta)stable thermodynamic phases in metals and transitions between them.

Steels, in particular, are characterized by a large variety of phases. Observed lattice structures vary as a function of temperature, composition and applied stresses. In addition, the magnetic order is closely related to structural properties. Phase separations, the formation and motion of grains and the inclusion of precipitates are essential for the mechanical properties of these materials. The stiffness and ductility of modern steels, such as those showing the TRIP and TWIP effect, is governed by martensitic transitions and the coexistence of lattice structures. For a tailoring of all these properties within the production process, it is vital to have a microscopic understanding of the underlying physics for the complete temperature range from the ground state to the melting point.

A key quantity to address such questions are free energy surfaces: The minima of such surfaces provide information regarding the thermodynamically stable phases while the low energy paths between minima provide information regarding the kinetics of the phase transitions. In order to accurately compute free energies ab initio simulations employing density functional theory (DFT) are performed. Since this approach is free of adjustable or empirical fit parameters it is principally well suited to predict thermodynamic quantities/phase diagrams for materials that are experimentally difficult to access. In order to test the suitability and the predictive power of this approach, the group has pursued the following activities: (i) Identification of an accurate and efficient DFT code for describing Fe-containing alloys. (ii) Development of an efficient approach to calculate thermodynamic quantities based on the DFT results. (iii) Benchmarking the predictive power by performing extremely accurate calculations for simple metallic systems.

A major research focus of the group has been on an ab initio treatment of those temperature dependent contributions to the free energy, which are due to lattice vibrations. The quasiharmonic approximation is used to determine the phonon excitation energies, which enter thermodynamic potentials via the partition function. As a result, thermodynamic properties such as lattice expansions and heat capacities can be obtained. The high predictive power of this approach can be seen in Fig. 2 by comparing theoretical predictions (dashed line; p=0 GPa) and experiment. To extend this formalism to magnetic systems, entropic effects due to spin excitations have to be considered. Therefore, using non-collinear spins also magnetic excitation energies will be investigated, by setting up frozen magnons and treating them similarly to phonons. As an alternative approach, magnetizations and Curie temperatures shall be obtained by studying model Hamiltonians (Heisenberg model, Kondo-lattice model) based on ab initio input. [2]

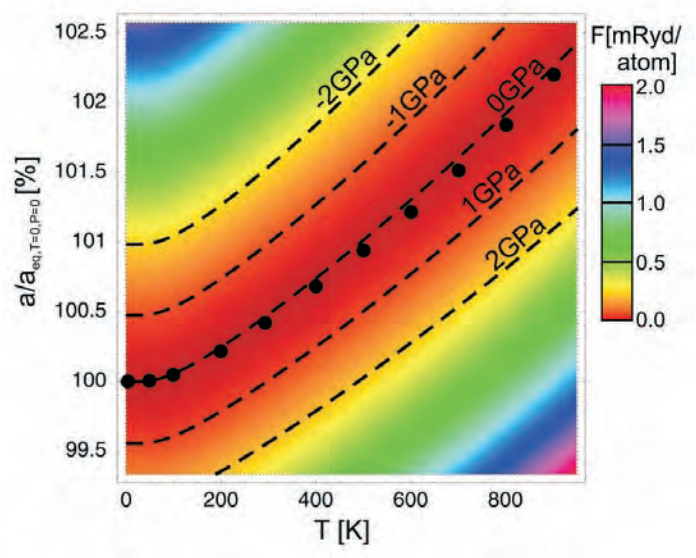


Fig. 2: *Free energy surface of aluminium as a function of the lattice constant a and temperature T. The lattice constant is given relative to the equilibrium lattice constant at T=0 and p=0 labelled* $a_{eq,T=0,p=0}$. *The free energy F (represented by the colours) is referenced to the p=0 free energy at each temperature. The dashed lines represent calculated thermal expansions at the given pressures. The dots correspond to experimental results for the expansion.*

The quasiharmonic approximation has been extensively tested for a large set of nonmagnetic, metallic elements. A comparison with available experimental data revealed a surprisingly good accuracy of the phonon spectra as well as of the thermodynamic properties. The analysis allowed the identification of some numerical problems, the improvement of the computational strategies and the discussion of chemical trends. Additionally, the temperature dependence of the free energies showed an excellent agreement with those obtained from ThermoCalc calculations (see p. 191).

Shape memory alloys (SMA) are an exciting material system. Similarly to steels, their mechanical properties are closely related to martensitic phase transitions, however their phase diagram is much less complex. Considering magnetic SMAs, these materials allow a systematic investigation also of magnetic contributions to the temperature dependence of the free energy. Therefore, the Heusler alloys (in particular Ni_2MnGa, a

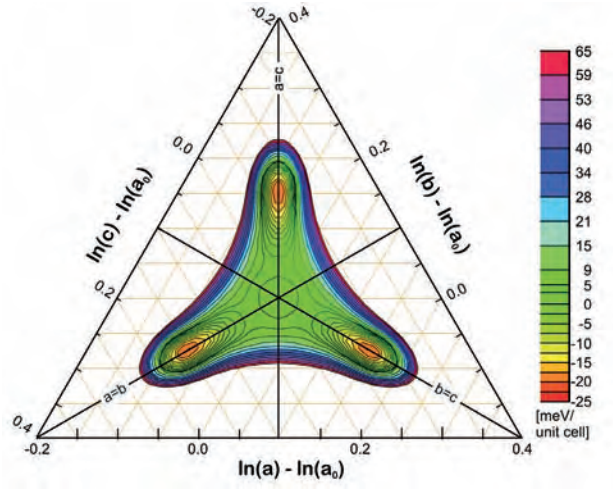


Fig. 3a: *Density plot of the total energy surface of the magnetic shape memory alloy Ni_2MnGa as a function the orthorhombic lattice constants a, b and c, where $a_0 = 5.81$ Å. The minima correspond to the austenitic cubic structure and the tetragonally distorted martensitic variants.*

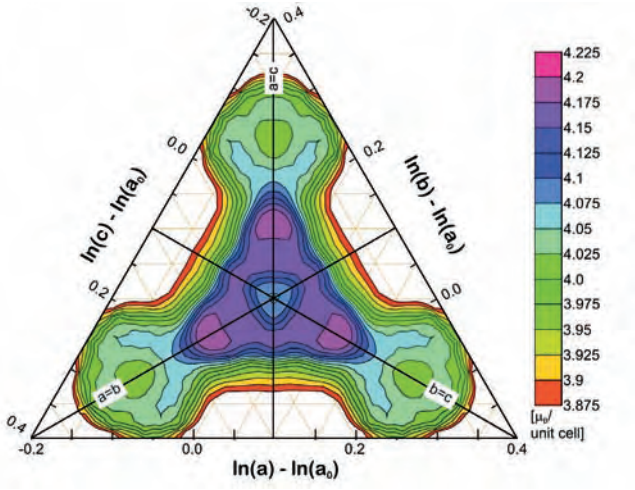


Fig. 3b: *Magnetic moment per unit cell of Ni_2MnGa. The calculations are performed for identical sets of lattice constants as used in Fig. 3a for the total energy calculations.*

prototype for a magnetic SMA) form another major research field of the group "Computational Phase Studies". The study of these materials is done in terms of free energy surfaces (see Fig. 3), spanned by lattice parameters (lattice constants, angles, volume). Soft phonon modes obtained in the quasi harmonic approximation are extensively used to determine the low symmetry shuffling structures, which are represented by local minima on this surface. The aim is a prediction of transition paths for the martensitic phase transition and transformations between martensitic variants as a function of temperature, magnetic field and composition. This research is embedded in a priority program (SPP 1239) of the DFG and benefits from intensive local, national and international collaborations.

Ab initio Thermodynamics (M. Friák)
(since June 2005)

The properties of materials are determined by their chemical composition and crystal structure. The prime focus of the group is the determination of the stability of different phases present in materials. Both, thermodynamic and mechanical properties are studied and the limits of stability are theoretically predicted. A combination of state-of-the-art techniques is used to achieve this task. First, methods based on fundamental quantum mechanics such as density functional theory are used to calculate the properties of selected ordered compounds on the atomistic level. Second, effective up-scaling towards macroscopic systems is performed employing the cluster expansion technique. This method expands materials characteristics into a series containing parameters assigned to specific atomic clusters. Any configuration-dependent property may then be fast evaluated even for systems containing millions of atoms, i.e. far beyond capabilities of current ab initio calculations. The results from the atomistic level are further passed on up-scale and used as input for phenomenological thermodynamic modeling employing the CALPHAD approach.

The main outcome of the research is a comprehensive understanding of materials characteristics with respect to the compositional trends and structure. The information will lead to the development of new materials with optimized properties. The theoretical results are systematically checked by collaborative studies with the experimental departments within the institute.

Recent highlights

The initial phase of the research has been focused on three classes of materials, (i) light-weight Fe-Al alloys with anomalous volume-composition dependence, (ii) non-toxic Ti-Nb binaries with human-body-matched mechanical properties for medical applications, and (iii) a joint group activity on the crystalline form of chitin.

The first topic was addressed together with the experimental group led by Dr. Martin Palm from the Department of Materials Technology. One aim of this collaboration was to gain insight into an experimentally observed anomaly in the composition-volume dependence in Fe-Al alloys. Based on density functional theory it could be demonstrated that the anomaly is due to a magneto-volume instability. The instability is caused by a transition of the magnetic moment of the iron atoms from a high-spin to a low-spin state (see p. 125).

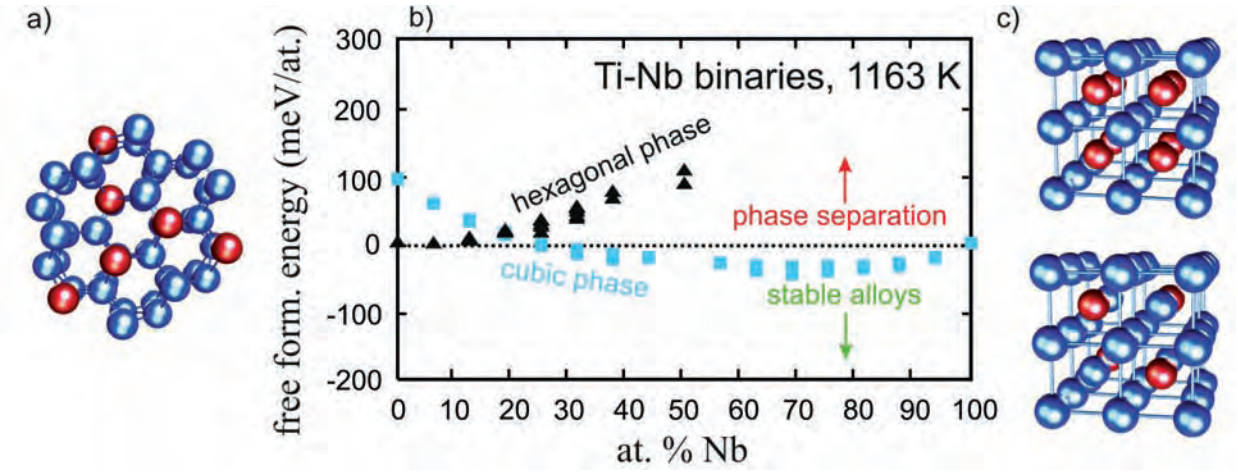


Fig. 4: *Alloy formation energies for binary Ti-Nb alloys as a function of alloy composition (b). The black and blue symbols mark results for the hexagonal close-packed (hcp) and cubic phase, respectively, exemplified on crystals in figures a) and c). The formation energies are shown at the temperature of the hcp-to-cubic transition in pure Ti (T=1163 K). At each concentration the formation energies of all supercells with that concentration but different local atomic configurations are given. The theoretically predicted composition range where the cubic phase becomes stable is close to the experimentally found value of 25 at. % Nb as minimum concentration.*

Another research activity was performed in close collaboration with experimentalists from the Department of Microstructure Physics and Metal Forming of Prof. Dierk Raabe. In this project a class of metastable Ti-alloys has been studied. This study is part of a current effort to design new implant materials with improved biocompatibility. The focus was on Ti-binaries containing exclusively non-toxic element (Ti and Nb). Employing density functional theory the thermodynamic stability of Ti-Nb binaries in the hexagonal and in the metastable cubic phase was calculated (see Fig. 4). Based on the calculated structures the Young module, which is the key quantity to characterize the mechanical biocompatibility with bone, was computed. The obtained relation between Young module and composition was used to guide the experiment (see also p. 125).

Microstructure (L. Lymperakis)
(since June 2005)

The microstructure group has the objective to identify and quantify the atomic scale mechanisms and structures which eventually determine the formation and evolution of the microstructure and thus the mechanical properties of a material. For this purpose, ab initio based methods are developed which allow to calculate structure, energetics and dynamics of extended defects such as dislocations and phase/grain boundaries.

The various activities of the group are highlighted in the following:

Ab-initio description of thermodynamically open systems

This approach is based on density functional theory and allows to derive the thermodynamic stability of thermodynamically open systems such as surfaces, interfaces, or extended defects as a function of the experimentally controllable conditions such as temperature, partial pressures, etc. In contrast to the thermodynamical activities in the previous two groups, phase diagrams as function of the chemical potential are studied here.

Development of ab initio based multiscale schemes to study extended defects

A major challenge in describing extended defects is the presence of long-range strain fields around the defective structure: The resulting structures are typically too large to be described directly by ab initio methods. Therefore, approaches have been developed which allow to partition the problem in spatial regions and to describe each region with an optimally adopted approach. For example, the core of a dislocation is described by density functional theory to accurately account for the broken bonds around the core, while the strain field around the core is described by a more approximate approach using empirical potentials. To connect the different regions a multiscale approach has been developed which connects density-functional theory, empirical potentials and continuum elasticity theory. The approach developed avoids explicit spatial boundaries between the methods but connects the

different methods via an implicit boundary scheme. A major advantage of this approach is that the region which needs to be described by the computationally expensive ab initio methods can be kept extremely small. The method has been first developed for dislocations and was extended over the last year to describe grain boundaries.

The new method has been successfully employed within the VIVIMAT project, a joint project between various institutes from the Helmholtz association, universities and the MPIE to develop multiscale strategies for casting and processing Al based alloys. A key quantity needed in this project was the grain boundary energy as function of grain orientation and inclination angle (see Fig. 5). Grain boundaries (GBs) play a key role in grain growth and recrystallization, and significantly affect the physical and mechanical properties of materials. Therefore, an important topic in materials design is grain boundary engineering, i.e. optimizing the population of GBs with desirable geometry by suitable thermomechanical treatment. Employing the implicit boundary scheme it became possible to map the entire five-dimensional configuration space. (see p. 150) The energies are now parameterized and will be used as input for mesoscale calculations.

Activities on III-Nitride semiconductors

The leader of the group, L. Lymperakis, has worked before his appointment at the MPIE on group-III nitride semiconductors. These semiconductors are the materials of choice for optoelectronic applications (LEDs, laser diodes - LDs, UV detectors) in the blue and ultraviolet regime of the optical spectrum. The studies sparked a lot of interest in the community and several projects funded by the DFG and EU have been awarded.

In one of these projects the focus is on the electronic and optical properties of semiconductor nanostructures (quantum dots) [3]. The zero-dimensional nature of these structures allows the design of novel high performance optoelectronic devices. A crucial aspect in the design and optimization of such devices is a detailed and predictive understanding of the electron and hole bound and wetting layer states and of the corresponding Coulomb matrix elements. Therefore, an efficient toolkit to calculate these quantities has been developed based on the S\PHI\nX library (with O. Marquardt, T. Hickel). Since the quantum dots embedded in the semiconductor matrix are highly strained the inclusion of elastic distortions turned out to be crucial. Therefore, based on DFT and the Special Quasirandom Structures (SQS) approach the second and third order elastic constants and band gaps of AlN, GaN, and their binary alloys have been computed. Although those calculations have been performed for a semiconductor, the formalism and the methodology behind them (anisotropic elasticity theory and modelling of random alloys) is universal and ready to be applied to metallic alloys.

Further Areas of Scientific Interest

Several funded projects and PhD studies, supervised by the department head Prof. J. Neugebauer, had been started before the opening of the CM department. Some of these projects have been integrated in these groups and are described in the corresponding group report. Examples are the nitride

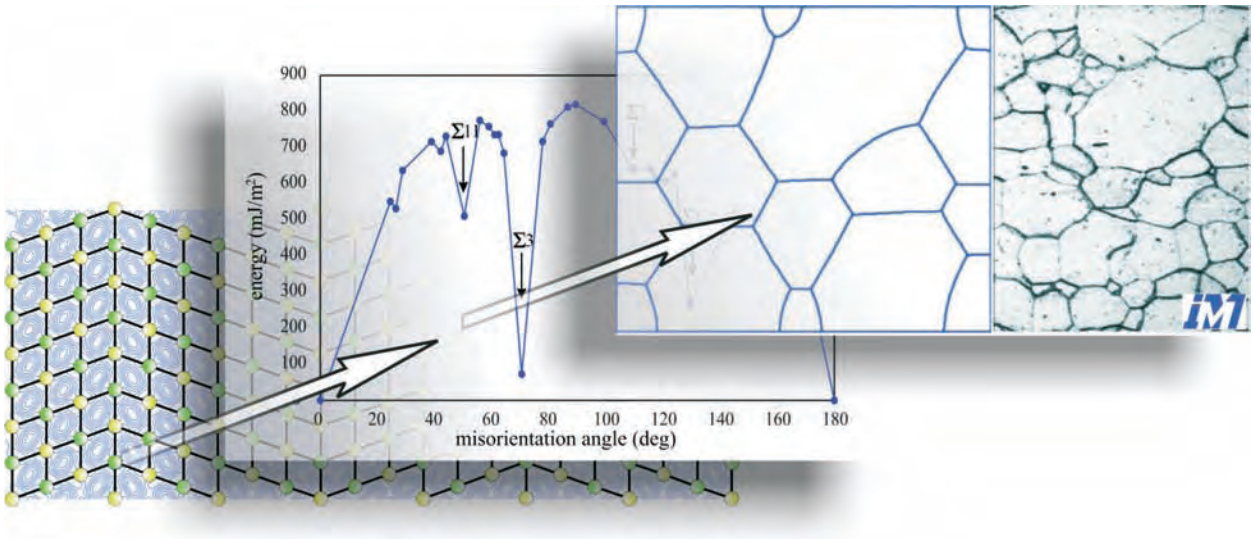


Fig. 5: *Multiscale approach to describe grain growth (schematic). Bottom layer: Employing an ab-initio based Implicit Boundary Scheme (IBMS) the full 5D configuration space of Grain Boundaries can be studied. Middle layer: The calculated Grain Boundary energies are needed as input for mesoscale grain growth simulations within the VIVIMAT project. The topmost picture shows the simulation of a 2D grain growth simulation (left) and the experimentally measured quasi-2D microstructures (right) as obtained from the Institute of Physical Metallurgy and Metal Physics RWTH-Aachen (Prof. G. Gottstein).*

activities performed in the Microstructure group. Other activities, which are briefly described below, have been performed outside the group structure. Although organizationally not directly related to the groups, the methods and expertise developed in these activities have been intensively used and significantly contributed to the methodological and scientific competence of the department. A few of these activities may serve as nucleus for a new research group.

Ab initio analysis of advanced scanning tunnelling microscopy techniques (A. Dick)

Scanning tunnelling microscopy (STM) has proved to be a valuable technique for the detailed study of various aspects and properties of surfaces down to the atomic scale. Recent extensions of this approach now allow to resolve surface magnetic structures on the nanoscale (spin-polarized STM) as well as the electronic structure (dispersion) of surfaces (Fourier transform STM). In the course of this project tools based on the S\PHI\nX package have been developed which allow an accurate and parameter-free simulation of both techniques. An example of the predictive power of this approach is shown in Fig. 6. Combining these techniques with experiments performed at the Ohio State University (Prof. A. Smith) and at the Fritz-Haber-Institut (Prof. K. Horn) a variety of hitherto not understood phenomena could be explained. [4,5,6] For example, for FT-STM an operational mode has been identified which allows to scan not only the dispersion of surface but also of bulk electronic states. For a detailed discussion of SP-STM, see p. 169.

Controlling bulk properties by surface engineering (H. Abu-Farsakh)

The properties of materials are often limited by thermodynamic constraints. An interesting option to overcome these limitations is to prevent the system from getting into its thermodynamically most stable state, i.e., to apply kinetic concepts. The aim of this project was to study how solubility of foreign atoms in crystals can be enhanced by employing surface engineering on the atomic scale. [7-10] The example studied here was on diluted nitrides (a few percent of N dissolved in GaAs) where the rather low solubility of N is a severe limit. This materials system has properties, which make it very appealing for the fabrication of infrared laser diodes as needed e.g. to optimize local area network communications. The ab initio based techniques developed and applied in this approach allowed to identify (i) surfaces which maximize the solubility of N, (ii) epitaxial growth conditions which stabilize these surface structures, and (iii) the kinetic processes which allow to prevent an equilibration between surfaces and bulk (see Fig. 7). In a joint collaboration between the institute for crystal research (Dr. M. Albrecht) and Infinion (Dr. H. Riechert) these theoretical predictions have been successfully used to interpret experimental data and to optimize samples.

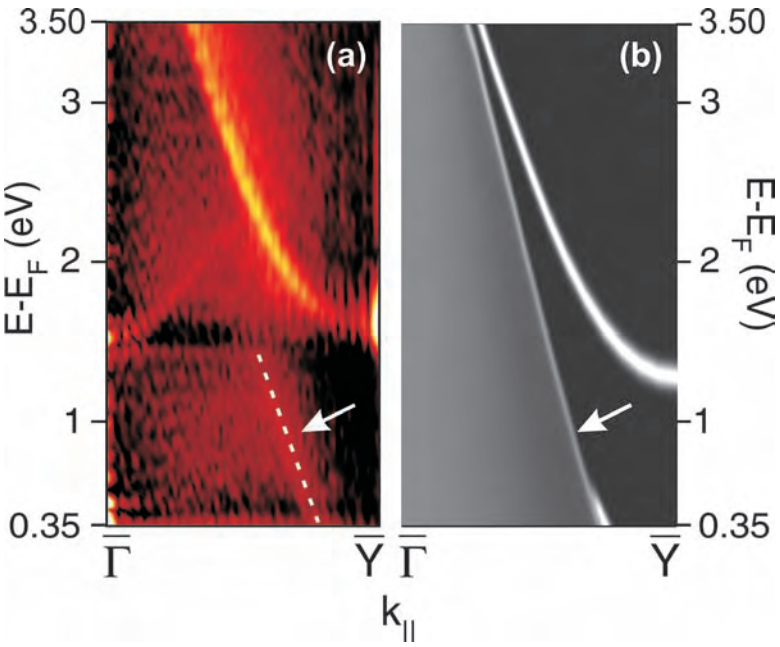


Fig. 6: *(a) Low temperature Fourier-transformed scanning tunneling microscopy (FT-STM) spectrum measured on a terraced Ag(110) surface and (b) the corresponding theoretical spectrum calculated from first principles. As expected for a surface sensitive technique the surface band (parabola with minimum at Y) is clearly visible. The ab initio simulations revealed that this technique can be extended to probe also bulk electronic states [arrows in a) and b)].*

Development and application of the Exact Exchange Functional in DFT (M. Wahn)

A well known deficiency of conventional DFT calculations employing the local density approximation (LDA) or the generalized gradient approximation (GGA) is the band gap problem: Calculated band gaps are significantly smaller than the experimental one and the predictions can fail even qualitatively. A prominent example is InN, a semiconductor which has a negative band gap in LDA and GGA, i.e., it is predicted to be metallic. A major source for the discrepancy between theory and experiment is the incomplete compensation of the spurious electron self interaction in LDA/GGA. To overcome this limitation, the Exact-Exchange Formalism (EEX) in DFT which is free of any electron self-

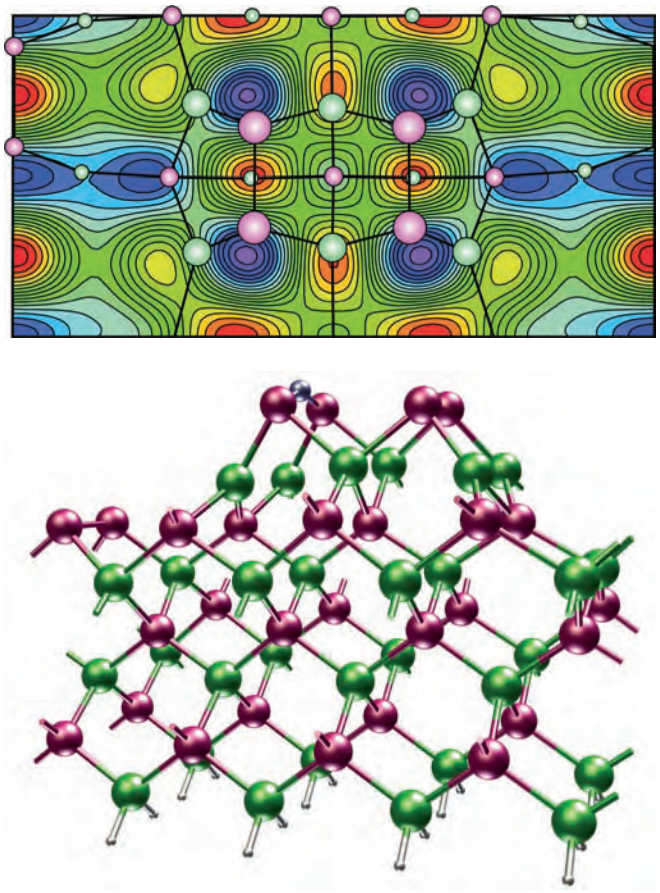


Fig. 7: *top: Contour plot of the potential energy surface of a N adatom on a GaAs β2(2x4) reconstructed surface. The color code and the contour lines (spacing 0.1 eV) give the binding energy of the adatom. The red/orange regions show the minima of the potential energy surface. Based on the total energy surface the adatom kinetics can be determined in detail: The global/local adsorption sites are given by the minima. The diffusion path and barriers can be obtained from the minimum energy paths. bottom: Schematic side view of the GaAs β2(2x4) surface. The As atoms are violet, the Ga atoms are green.*

interaction has been implemented in the S\PHI\nX library. [11,12] Since the original method turned out to be computationally extremely demanding a novel variational approach has been developed, implemented and successfully applied to study an extensive number of II/VI and III/V semiconductors. In order to further improve the description of the electronic structure the EXX results have been used as input into GW quasiparticle calculations in a joint collaboration with the Fritz-Haber-Institut (Prof. M. Scheffler, Dr. P. Rinke) and the Yarmouk university in Jordan (Prof. A. Qteish). The joint EXX and GW approach was found to systematically provide bandgaps with error bars < 0.1 eV. [13,14] The approach has been recently used to derive an accurate tight binding parameterization employing maximally localized Wannier functions to describe the electronic states in semiconductor nanostructures. [15] A possible application of these methods for the new research areas is an improved description of oxide surfaces and interfaces as relevant e.g. in the Interfaces and Surfaces Department (Prof. Stratmann).

Ab initio thermodynamics of small biomolecules (L. Ismer)

As in engineering materials, temperature driven phase transitions may have severe consequences for the functionality and stability of biomolecules. In order to obtain a detailed understanding how temperature affects the stability of the basic secondary motives (such as e.g. helices) tools to compute the free energy of these structures with high accuracy (resolution of the phonon frequencies < $3cm^{-1}$) are needed. [16] The simulation tools developed in this project are based on DFT theory and the quasiharmonic approximation. [17] For some of the structures the harmonic approximation was found to be insufficient and anharmonic contributions had to be included. Therefore, an efficient scheme to calculate anharmonic contributions by thermodynamic integration and Langevin dynamics has been implemented in S\PHI\nX. Based on these results it could be explained why poly-alanine is a good helix former while poly-glycine not, why the π-helix is stable at T=0K but not at room temperature, as well as how the cooperative character of the hydrogen bond networks affects the temperature dependence. The methods to study anharmonic entropy contributions developed and implemented in this project will be transferred to the Computational Phase Study group to investigate metallic materials.

Bioinspired materials (M. Petrov, M. Friák, L. Lymperakis)

Many of the structures "invented" by nature exceed in many respects man made materials. There is therefore a strong interest to learn how nature designs materials and how these principles might be used to construct new engineering materials. A bio-composite, which has been studied intensively experimentally in the Leibniz group of Prof. Raabe is chitin. The complex microstructure of chitin results in a low-weight and high-strength material. Additionally, chitin is characterized by unique chemical properties (non-toxic, non-allergenic, anti-microbial, and biodegradable) which are of great interest for medicine and pharmaceutical applications. In order to understand the interplay between the mechanical properties on the nanoscale and the complex microstructure, which eventually results in the fascinating properties of chitin, it is crucial to develop a detailed

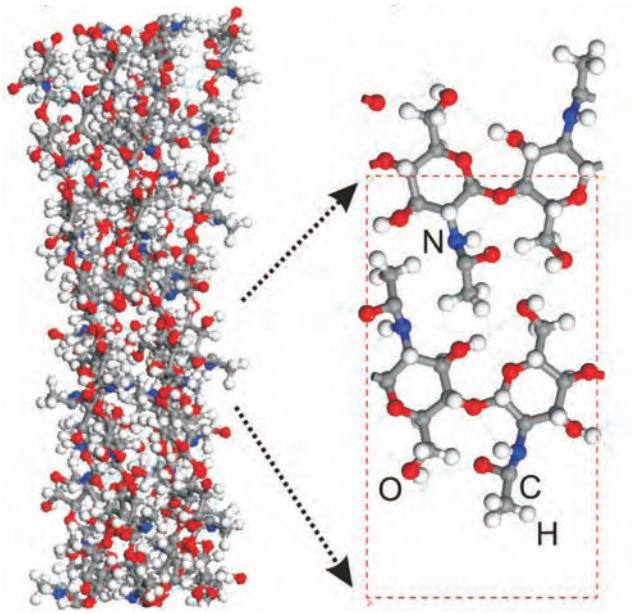


Fig. 8: *Chitin shell of arthropods, as e.g. lobsters, represents an example of natural materials design resulting in a complex lamellar exoskeleton with unique mechanical properties. The structure can be hierarchically decomposed into layers, microfibrils (left) and ultimately into the smallest building units consisting of 108 atoms (right). Employing DFT the atomic structure of single crystalline chitin has been determined.*

understanding of the elastic properties on the nanoscale. This information is experimentally not accessible. Therefore, the aim of this project is the determination of the atomic structure of single crystalline α chitin (see Fig. 8) and based on this information to derive the elastic parameters. To perform this task a series of hierarchical approaches/ methods is used: A conformational analysis of chitin is performed using computationally fast empirical potentials and tight binding calculations. Based on the conformational analysis a small number of possible atomic configurations could be identified. These structures have then been used as input for accurate ab initio calculations in order to derive the ground state atomic geometry and the elastic properties of chitin. The thus obtained data will be used as input for mesoscale simulations in the department of Prof. Raabe.

Large scale simulations of defect dynamics and grain growth (Dr. J. von Pezold)

Very recently (Nov 1, 2006) a new activity started which is devoted to bridge the simulation activities between the ab initio based studies in the CM department (Prof. J. Neugebauer) and the crystal-plasticity FEM approaches in the MU (Prof. D. Raabe) department. In this activity approximate empirical potentials will be used to perform large scale calculations to study the kinetics and the interaction of dislocations and grains. The results will be used to validate the approximations employed to derive the constitutive equations in the crystal plasticity approach and to derive microscopic parameters.

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Research Projects in Progress

Algorithm Design and Modelling

Boeck, Neugebauer: S/PHI/nX – The ab initio based multi-scale library

Bubnik, Uchdorf, Wellms, Boeck: PHInaX – Development of a cross-platform visualization package

Bubnik, Boeck: Interactive 3d visualization of electronic charge densities

Boeck, Neugebauer: Thermodynamic properties of semiconductors

Computational Phase Studies

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

Grabowski, Hickel, Neugebauer: Ab initio based modeling of thermodynamic properties and martensitic transformations in metals

Marquardt, Hickel, Neugebauer: Multiscale growth and doping simulations of nanostructured devices, *in collaboration with Jahnke*, Czycholl* (*Univ. Bremen)*

Ismer, Hickel, Neugebauer: First-principles Studies of Hydrogen in Metals, *in collaboration with Van de Walle* (*Univ. of California, Santa Barbara, USA)*

Hickel, Neugebauer: Prediction of structures and phase diagrams in solid state chemistry, *in collaboration with Jansen*, Schön* (*MPI-FKF, Stuttgart)*

Grabowski, Neugebauer: Kinetic, structural and dynamic properties of the phase change alloy $GeSb_2Te_4$, *in collaboration with Lencer*, Wuttig* (*RWTH Aachen)*

Todorova, Hickel, Neugebauer: Ab initio study of corrosion: Adsorbate phases on surfaces and phase diagrams, *in collaboration with Grundmeier* (*MPIE Düsseldorf)*

Ismer, Hickel, Neugebauer: Ab initio thermodynamics and kinetics of the material system Fe-Mn-C (in preparation)

Hickel, Neugebauer: Ab initio simulation of diffusion processes in the W/steel hybrid system, *in collaboration with Aktaa* (*FZ Karlsruhe)* (in preparation)

Hickel, Neugebauer: Verification of empirical potentials using ab initio methods, *in collaboration with Moseler* (*IWM Freiburg)* (in preparation)

Ab initio Thermodynamics

Friák, Neugebauer: Cluster-expansion calculations of Fe-Al alloys, *in collaboration with Müller* (*Univ. Erlangen-Nürnberg)*

Friák, Neugebauer: Phase stability and mechanical properties of biocompatible Ti-alloys, *in collaboration with Raabe* (*MPIE Düsseldorf), Šob** (**Masaryk University in Brno, Czech)*

Friák: Ab initio calculations of structural and magnetic phases of iron, *in collaboration with Šob* (*Masaryk University in Brno, Czech)*

Kim, Friák: Thermodynamic assessment of the Fe-C system employing the CALPHAD and ab initio methods, *in collaboration with Schneider* (*RWTH Aachen)*

Microstructure

Lymperakis, Neugebauer: Implicit Boundaries Multiscale Scheme Calculations of grain Boundaries in Aluminum

Lymperakis, Neugebauer: Nitride based quantum dot lasers

Petrov, Lymperakis, Neugebauer: Ab-initio calculations of III-Nitride semiconductors

Lymperakis, Neugebauer: Ab-initio study of AlN growth and doping efficiency, *in collaboration with Albrecht* (*IKZ Berlin)* (in preparation)

Joint group activities

Grabowski, Lymperakis, Neugebauer: Theoretical and experimental multiscale modelling of Al and $AlCu_4$, *in collaboration with Mohles*, Gottstein* (*RWTH Aachen)*

Petrov, Lymperakis, Friák, Neugebauer: Atomistic calculations of the mechanical properties of chitin molecules, *in collaboration with Raabe* (*MPIE Düsseldorf)*

Dick, Neugebauer: Ab initio based analysis of spin-polarized scanning tunnelling microscopy

Abu-Farsakh, Neugebauer: Enhancing the solubility of N in GaAs and InAs by surface kinetics

Ismer, Neugebauer: Vibrational and thermodynamic properties of regular secondary structure motifs

Wahn, Neugebauer: Exact Exchange Functionals in DFT

von Pezold, Neugebauer: Ab-initio simulation of lattice defects in metals, *in collaboration with Raabe* (*MPIE Düsseldorf)*

Department of Interface Chemistry and Surface Engineering

M. Stratmann

Introduction

The department mainly focuses on chemical reactions and physical properties of surfaces and interfaces with particular emphasis to increase their stability and to include functional properties into coatings on structural materials. The material classes of particular interest include metals, polymers, ceramics and their composites. Scientific studies related to these materials in particular concentrate on degradation reactions such as aqueous corrosion, high-temperature corrosion, tribocorrosion and de-adhesion reactions with the aim to understand their underlying physico-chemical reaction mechanisms. Based on this knowledge new and superior surfaces and interfaces are designed, characterised by their novel chemical composition, morphology and molecular and atomistic structure. Frequently, this requires the application of new surface modification techniques. The physico-chemical understanding of such technologies with regard to their application in tailoring surface and interfaces complements the analytical approach of the department.

Currently, the department includes approximately 65 people and among them more than 45 scientists working on more than 30 projects – most of them integrated in international collaborations with scientists in Europe, Asia and the United States. The experimental equipment is exceptional even on an international scale and allows performing state of the art science in surface and interface chemistry.

The structure of the department is summarised in Fig. 1. This structure includes three major lines:

i. *Scientific groups* as the most important part of the management structure. These groups are competence centres in various areas of science and they include specific experimental and theoretical knowledge. The scientific groups are largely integrated in the major departmental fields of scientific interests; however in parallel they also have their own specific and unique scientific goals.

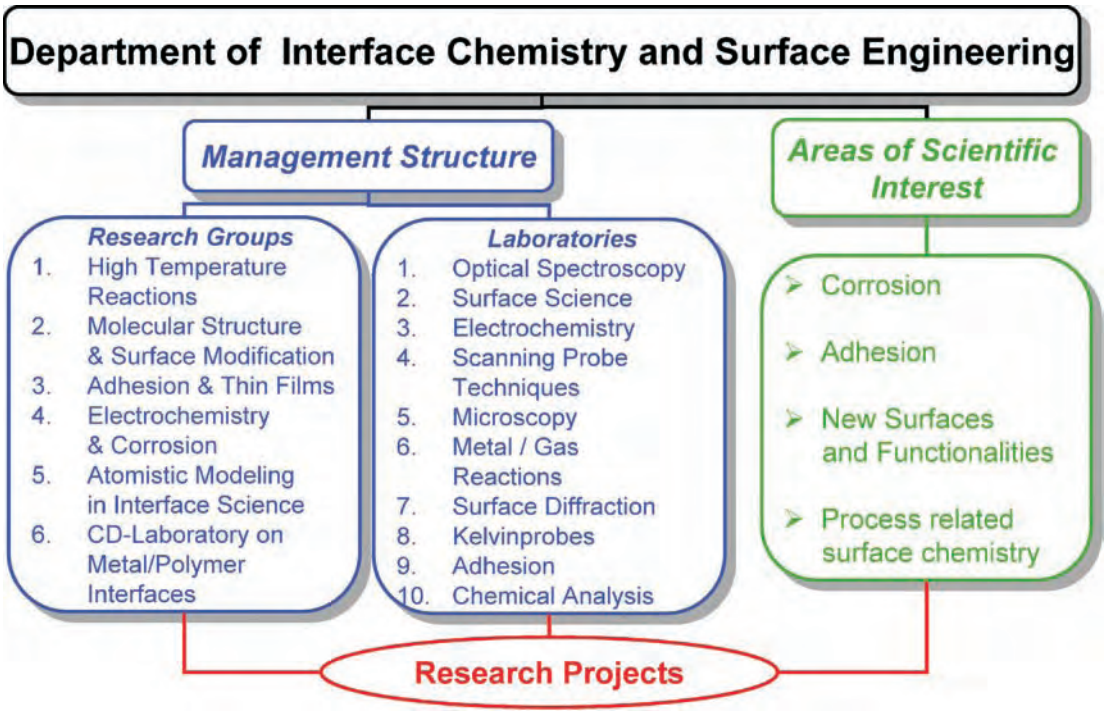

Fig. 1: *Organization of the Department of Interface Chemistry and Surface Engineering.*

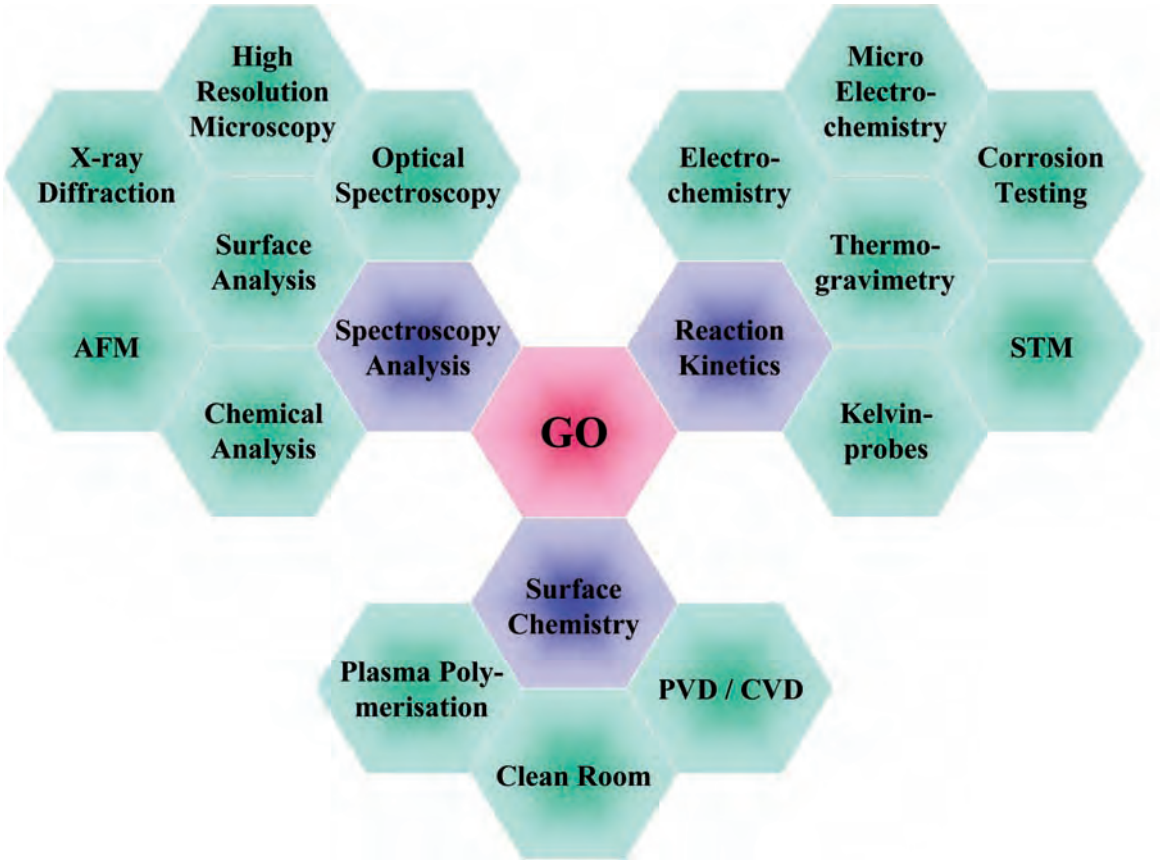

Fig. 2: *Experimental laboratories of the Department of Interface Chemistry and Surface Engineering.*

ii. *Laboratories (Fig. 2)* include the experimental techniques necessary for investigating surfaces and interfaces. Besides serving the scientific groups for their experimental needs they serve as centres for the development of new and often unique experimental set-ups as a prerequisite for many state of the art research projects. Obviously, there exist strong links between the specific experimental knowledge of the scientific groups and some of the key laboratories.

iii. The department has clearly defined *areas of scientific interests* which are common for almost all scientific groups and which define a scientific link between them. Indeed, the long term goals on which the areas of scientific interests are based, can be achieved only if the groups of differing scientific knowledge strongly collaborate. The collaboration is organised in short term projects typically financed either by scholarships or by European or German funds.

The department is well integrated into the scientific structure of the institute. Major links include aspects of micromechanics of surfaces, interfaces and thin films (Prof. Raabe), the correlation between the reactivity of surfaces and their microstructure (Prof. Raabe), the corrosion stability and surface characteristics of novel materials after heat treatment and the formation of novel microelectrode arrays (Prof. Frommeyer), the use of synchrotron radiation as powerful analytical tool (Prof. Pyzalla) and an intense collaboration with Prof. Neugebauer in areas like hydrogen in steel or semiconducting oxides. The atomistic scale of many experiments within the department is very much in line with the computational expertise of Prof. Neugebauer's department.

Finally, it should be mentioned that the department is highly dedicated to activities beyond the institute. The department coordinates a number of European research projects, it has attracted a *Christian Doppler Laboratory on Polymer/Metal Interfaces* financed by the Austrian CD-Society (Head of the CD-Lab: PD Dr. Guido Grundmeier) and based on its initiative the IMPRS "*SurMat*" has been founded, which nowadays acts as a major source for international PhD students.

Scientific Concepts

All scientific groups are horizontally linked by common areas of scientific interest:

Corrosion

Research of the department includes aspects like aqueous corrosion, atmospheric corrosion, flow induced corrosion, microbially influenced corrosion [1], corrosion inhibition and high temperature corrosion. Aspects which have been of considerable importance for the department over the last 6 years are:

- *Corrosion studies of novel materials with considerable technological importance* like TRIP and TWIP steels, iron-aluminides [2], shape memory alloys [3,4], novel Ni-free Cr-based stainless steels [5] etc.
- *Understanding of corrosion reactions on a microstructure scale* taking into account the influence of the grain orientation and the grain boundary structure on the local corrosion kinetics [5,6]. This includes aqueous or atmospheric corrosion phenomena where local electrochemical techniques such as SKPFM [7] and microelectrodes [8] are being used as well as novel experimental tools for high temperature corrosion where the nucleation and growth of oxide scales is studied in-situ within a SEM chamber making use of the EBSD technique for the identification of individual grains and grain boundaries [9].
- *Understanding of corrosion reactions from an atomistic to a macroscopic scale* in particular for high temperature corrosion reactions. The very first stages of alloy oxidation are studied in-situ by high temperature STM, the formation of first 3D nuclei by the combination of SEM, a reaction chamber and EBSD and the formation of oxide layers by synchrotron based x-ray diffraction and a home-built high pressure reaction chamber within a complex UHV analytical system.
- *Optimisation of corrosion resistant surfaces by combinatory materials science.* Graded alloy surfaces are being prepared using multi-component PVD techniques and subsequently studied by localised fast screening techniques. These are for aqueous corrosion the scanning electrochemical droplet cell and for atmospheric corrosion the scanning Kelvinprobe. Similar approaches will in future be realised for the high temperature corrosion probably using Raman microscopy as local analytical probe.
- *Combination of experiment and theory* is still a challenge for complex reactions like corrosion reactions. Nevertheless in the future there will be a strong focus on applying ab-initio calculations on simple corrosion systems in collaboration with the department of Jörg Neugebauer. This will include the study of H-permeation and H-trapping in steels, the study of electronic properties of passive films formed on alloys like Zn-Mg as well as studies on surface segregation of non-metals upon heat treatment.

Adhesion

As a consequence of the invention of the scanning Kelvin probe by M. Stratmann and co-workers the study of buried metal/oxide – polymer interfaces is a prime target of the department. This technique has proven to be most powerful in studying even elementary reactions which lead to the de-adhesion of polymers from solid surfaces in aggressive media. Typical applications are de-adhesion processes of polymers from electronic circuits during the pressure cooker test, the delamination of paints from metallic substrates and the de-adhesion of glues in structural joints.

Research concentrates on the following issues:

- *New analytical instruments.* The department has succeeded in building up a 3D-scanning Kelvin probe which now also is available as commercial instrument in a spin-off company. This new instrument has also been complemented with a blister-test to study for the first time de-adhesion reactions under combined electrochemical and mechanical load [10]. In addition the scanning Kelvin probe force microscopy is established as a novel technique.
- *Mobility of water and ions along the buried interface.* Both mobilities are studied by means of in-situ vibrational spectroscopy and the scanning Kelvin probe. The latter allows the detection of a change in the charge of dipole distribution at the interface. Both methods also allow differentiating diffusion along the interface from bulk diffusion. Results have shown a surprisingly strong dependence of the interfacial mobility on the interfacial structure [11].
- *Electrochemical and chemical reactions at the buried interface leading to de-adhesion*. Besides the scanning Kelvinprobe UHV-based spectroscopic techniques such as ToF-SIMS [12], also optical techniques are increasingly used to understand details of the dominant de-adhesion reactions. The rate of the electron transfer depends critically on the electronic

properties of the oxides being present at the interface. Inherently stable interfaces have been designed by optimising the oxide defect structure such that the work function of the oxide covered metal/polymer interface matches the work function of the freely corroding iron surface (system Zn-Mg) [13].

- *Chemical bonds at the buried interface*. Obviously chemical bonds are essential for creating stable composites. The department had considerable success in the development of the self assembled monolayer concept for adhesion promoters used on technical surfaces [14]. In particular phosphonate based molecules have been developed for Al-oxide terminated surfaces and a successful industrial surface treatment is based on the application of this technology (Chemetall). The formation and breaking of chemical bonds is studied by optical techniques but also for the first time using single molecule interactions by an AFM equipped with an electrochemical cell [15].
- *Theory*. As the experimental access to buried interfaces is clearly limited a strong aspect of future research lies in the theoretical understanding and modelling of chemical bonds, mobility of ions, electrochemical reactions etc. at the interface. Therefore a new group has been established recently in this direction with a specific emphasis on chemistry using DFT based techniques. This group closely interacts with the experimental groups which will have to provide critical experiments for validating theoretical predictions and with the theory department of Jörg Neugebauer.

Functional surfaces and interfaces

The department has a considerable interest in the study of new function surfaces and interfaces aiming to combine traditional aspects of organic coatings like adhesion or corrosion protection with novel aspects. Within the last years physical and chemical vapour deposition as well as colloid chemistry have been of particular interest:

- *Plasma surface oxidation and reduction.* Oxidising and reducing plasmas at reduced and atmospheric pressure are employed as a measure for the tailoring of passive films on metal alloys (e.g. $MgZn_2$) and the introduction of chemical groups in model polymer films [16].
- *Plasma polymer composite films*. By combining PVD of Ag and plasma polymerisation of fluorinated monomers, model metal/polymer nanocomposite films could be designed which allow a detailed analysis of the release properties of Ag-nanoclusters in a perfluorinated matrix. A recently developed co-sputtering unit allows the integration of Ag-nanoparticles in semiconducting oxides for applications as antibacterial or photochromic films. Moreover, corrosion resistant thin films are developed for galvanised steel sheets with the focus on the understanding of the possibility to adjust interfacial electrode potentials.
- *PVD coatings.* These coatings are of considerable interest on steel and galvanised steel substrates. They are either used to form tailored oxides with a specific electronic structure or they are used for surface alloying. Surface alloying is regarded as a most interesting topic for the formation of patinas on steel and recent research concentrates in particular on the reaction mechanism of patina formation making use of spectroscopic and Kelvin-probe methods.
- *Smart interfaces with self repair properties*. The scanning Kelvin probe has shown, that the local electrode changes dramatically upon de-adhesion of the polymer film. This observation is used in the development of composite coatings containing nanoparticles of conducting polymers [17-20]. Additionally, inorganic nanocapsules with intelligent release function are developed for embedding either in the polymer matrix or even within galvanic alloy deposited zinc coatings. Both systems release surface active ions being able to stop corrosion reactions at the defect interface upon change of the electrode potential. These systems under investigation are the first ones which clearly demonstrate, that self repair of defects is possible, if the underlying electrochemistry is clearly understood.

Process-related surface chemistry

Steel surfaces are of particular interest for the department. In close collaboration with the steel industry and in many cases funded by European funds, steel related projects cover the full range of surface treatments which is of importance in nowadays steel surface chemistry.

- Short time annealing is studied to understand the scale formation prior to galvanising in oxidizing and reducing atmospheres. The segregation of non-metallic elements is of particular importance [21].
- Hot dip galvanizing is determined by wetting of liquid zinc on the oxide covered surface and by interfacial reaction between the liquid bath and the substrate. Both phenomena are studied with unique instrumentation.
- Surface reactions between zinc alloys and the gas phase lead to semi conducting oxides; this is subject of extensive investigations.

- Cleaning of the surface, phosphatising and in particular the deposition of chromate alternative coatings based e.g. on zirconates are studied in detail in particular with spectroscopic and electrochemical techniques [22-24].
- The interaction of water born coatings and pigments with steel and galvanised steel surfaces is being studied in close collaboration with the chemical industry [25,26].
- Adhesive bonding as one of the most promising joining technologies for multimaterials applications is studied with the focus on the understanding of the stability of interphases under corrosive and mechanical load.

Scientific Groups

1. High Temperature Reactions Group (PD Dr. M. Spiegel)

The research of the group is focussed on high temperature reaction phenomena of metals in the presence of gases, solid particles and melts. Of particular interest is the stability and electronic properties of high temperature oxide films, which are studied on model systems, in order to gain knowledge on mechanisms of oxide scale formation and breakdown as well as on semiconduction properties for application in fuel cells. This work is done in collaboration with the group 'Electrochemistry and Corrosion' (Dr. Hassel). Interest is paid to mechanisms of oxidation and segregation to metal surfaces upon short term annealing. This work is connected to the wetting studies, carried out in the group 'Molecular Structure and Surface Modification' (Dr. Rohwerder). Several short term annealing chambers have been developed and constructed, also for connection to the UHV system. Furthermore, the group has developed chambers for in-situ investigation in the FE-SEM connected with EBSD and EDX as well as for adoption to grazing incidence diffraction set-up at the ANKA synchrotron source. Future work is focussing on mechanisms of wetting of salts with oxides and metals, on the construction of a specific cell for studying oxide conductivity at high temperature in the presence of gases. Methods for measuring short term oxidation kinetics as well as for grain resolved segregation phenomena by means of AES will be developed in the next years. *Ab initio* simulation of non-metal segregation is a further task which will be studied in the future.

The main interests of the group are:

i. Mechanisms of high temperature corrosion in complex conditions and materials development

ii. High temperature oxide films

iii. Oxidation and segregation on steel and alloy surfaces upon short term annealing (see selected topic)

This activities are represented by the following topics:

1. Mechanisms of corrosion in thermal power plants

Fireside corrosion by combustion gases and ash deposits is the major limiting issue for the application of steels as heat transfer surfaces in thermal power plants. The role of alloying elements in the 'active oxidation' mechanism, a chlorine catalysed reaction cycle leading to enhanced oxidation via volatile metal-chlorides as intermediate products, was studied by using model systems [27]. It was found that chromium is not beneficial if its concentration exceeds 15 wt. % due to the formation of volatile $CrCl_3$. At temperatures lower than 400 °C, the adhesion and reaction of solid and especially molten salts on the metal surface is responsible for most of the corrosion phenomena. The group has established a corrosion model for the main elements Fe, Cr and Ni in a molten chloride salt. The model considers first the formation of metal-chlorides, which are subsequently dissolved in the molten salt i.e. high solubility favours high corrosion rates. Iron and especially chromium shows a high solubility, i.e. Cr as CrO_4^{2-} [28]. The investigations lead to the development of ferritic Fe-Al and Fe- 9 %Cr Al Si alloys, which form an alumina scale very quickly and show satisfactory corrosion rates. Salt particle adhesion most probably occurs by a liquid film, which forms between the particle and the metal [29].

2. Alumina scale growth at low temperatures

Alumina scales of corundum type passivate alloys at high temperatures due to its wide band gap and slow diffusion coefficients for Al and O. As there are rarely studies on alumina scale formation at temperatures of 600 – 800 °C, which is in contradiction to the urgent need of protective materials for energy conversion, alumina scale formation is studied on Fe-Cr-Al-Si alloys at a temperature of 700 °C. Surprisingly, only corundum and no metastable alumina phases were detected. Obviously, corundum is formed by using Fe_2O_3 and/or Cr_2O_3 as template structures rather than by nucleation and growth. This was proven by the oxidation of Fe-6Cr1Al1Si alloy. The oxidation

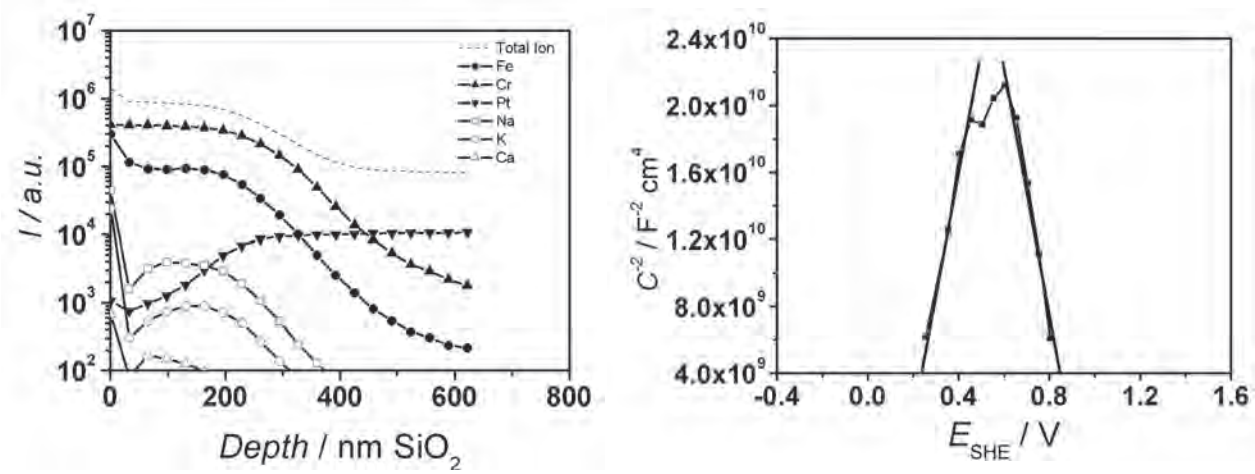

Fig. 3: *Chemical composition in the form of a ToF-SIMS sputter depth profile of the $(Cr,Fe)_2O_3$ model oxide on top of Pt (left). Corresponding Mott-Schottky-Plot of the oxide film in borate buffer solution at room temperature (right). The oxide shows n-type semi-conductive behaviour in the lower potential range and a p-type behaviour in the higher potential range.*

process goes through several distinctive steps. Initially a $(Fe,Cr)_2O_3$ was formed with a Fe enrichment at the outer part and Cr in the inner. Al then oxidises and dissolves into the Cr_2O_3 rich part. Al_2O_3 forms solid solutions with Cr_2O_3 but not with Fe_2O_3. Al is enriched in the oxide and can form a layer Al_2O_3 with minute amounts of Fe in the outer Cr in the inner part. The results offer a new way of explaining the so called third element effect. It is fact the $(Fe,Cr)_2O_3$ acts as a template for the $(Al,Cr)_2O_3$ which later develops into a Al_2O_3. Further work is now carried out on a basic understanding of the difference between corundum formation using a pre-cursor phase or by nucleation and growth. The correlation between oxygen surface potential and metastable alumina formation is studied in detail on single crystals of Fe-26Al by using high temperature electrochemical techniques, surface x-ray diffraction (cooperation with MPI-MF Stuttgart) and *ab initio* modelling.

3. Development of alloys forming conductive oxide scales for molten carbonate fuel cell applications

The molten carbonate fuel cell is running at 650 °C with molten carbonates as electrolyte. By oxidation of the metallic current collectors, usually made of stainless steels, insulating phases such as Cr_2O_3 and Al_2O_3 are formed, thus leading to potential drops. Spinel phases were found to be reasonable oxide systems, providing sufficient corrosion strength and conductivity [30]. As Fe_3O_4 is known to be a nearly metallic conductor, it is fast growing, thus leading to high corrosion rate. On the other hand $FeCr_2O_4$ provides slow growth rates but low conductivity. The strategy developed was based on incorporating multivalent ions, Mn, Co to the $FeCr_2O_4$ in order to increase its conductivity, i.e. enhance electron hopping by multivalent ions on similar crystallographic sites. The approach was proven by model alloys containing Fe-15Cr-Mn-Co with systematic variations in concentrations of Co and Mn. The electronic conductivity was measured in-situ during reaction within a carbonate melt. The lowest resistivity was measured for a Fe-15Cr-10-Co-2Mn alloy, which forms a Co-and Mn-containing spinel as a corrosion product. It was found that the spinel layer changed composition with time by outward diffusion of Co and Mn-ions. The studies are now focussing on fundamental studies of spinel systems, as prepared by PVD and subsequent oxidation.

4. High temperature oxide films for fuel cells

The intention is to prepare oxide films on top of Pt substrates and measure the conduction properties, first at room temperature and then at the higher temperatures and then to compare with films grown on steels. The first step has been to establish a reproducible and well controlled process to deposit Fe, Cr and Cr-Fe alloys and then thermally oxidize them in O_2 forming Cr_2O_3 and Fe_2O_3 and $(Cr,Fe)_2O_3$, which are all oxides with corundum type structure. The results from the preparation work can be exemplified by 200 nm $(Cr,Fe)_2O_3$, the chemical analysis of this oxide is shown in Fig. 3. EIS measurements and Mott-Schottky plot have been used in order to investigate the electronic properties. The results from the pure Fe_2O_3 and Cr_2O_3 oxides compared excellently with results reported in literature, which shows that our synthetic thermal oxides very well mimic an oxide formed “naturally” on Fe and Cr. The measurements on $(Cr,Fe)_2O_3$ gave complex though extremely interesting results. In the case of $(Cr,Fe)_2O_3$ a dual p- and n-type behaviour were observed which appeared as the potential was changed. This indicates a defect structure that differs completely from those of the pure oxides. The appearance of this double behaviour is quite often seen in the literature in Mott-Schottky

plots made on stainless steels, the presence of a double slope is however rarely commented on and is not explained by the presence of a $(Cr,Fe)_2O_3$ solid solution. Further work is now in progress on the preparation of spinel systems on platinum and steel substrates.

2. Molecular Structure and Surface Modification (Dr. 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. To this end, as a central tool for the preparation of dedicated model samples, a complex UHV system, features a number of different surface preparation and analysis techniques. The main vision for the medium-term future is to provide a detailed model for electrochemically driven coating delamination (in cooperation especially with the simulation group of Dr. A. T. Blumenau) and based on this to develop novel protection concepts.

The group's current main interests are focussed on:

i. elementary steps of electrochemical driven de-adhesion of polymers

ii. semiconducing properties of surface oxide films

iii. wetting and interfacial reactions at metal/metal melt interfaces

iv. intelligent self-healing concepts for corrosion protection

v. surface modification by organised monolayers

They are reflected in the following main activities:

1. Zinc and zinc alloy coatings

The electronic properties of the oxides formed on a metal during short term annealing or other pre-treatments define the rate of electron transfer reactions (ETR) at the buried interfaces. Fundamental studies performed in the group, which could be regarded as the surface physics group of the department, have demonstrated for the case of novel zinc alloy coatings that intrinsically stable interfaces can be formed, if the Fermi level within the oxide is tailored such that potential differences between defect and intact areas of the delaminating coating is inverted [13]. This finding, which is a breakthrough in interface chemistry, has triggered the start of fundamental studies on the electronic properties of buried interfaces. These studies include the preparation of well defined oxides in the integrated UHV system of the department, the study of ETR on metal/polymer interfaces with a given distribution of the potential making use of charged monolayers prepared by the Langmuir-Blodgett technique and the study of the chemical interaction between the substrate and organic molecules using e.g. scanning probe techniques (see fundamental studies).

The potential inversion observed for the case of $MgZn_2$ rich zinc alloy coatings is not observed for hot-dip prepared zinc alloy coatings with smaller contents of Mg. However, it could be shown that for such Zn-Mg-Al based coatings the oxide distribution, i.e. the surface microstructure, plays an important role for the delamination behaviour. At basically the same overall composition, the oxide distribution could be shown to have a significant effect on the delamination kinetics. The underlying mechanisms are still subject of current research.

The process of hot dip galvanising itself, i.e. the wetting and interfacial reaction at the metal/melt interface is another important research topic within the group. The problem are stable oxides such as alumina, silica or manganese oxides characteristic for highly alloyed steels (such as high strength steels) that cannot be removed in the reductive annealing step in forming gas atmosphere (95% N_2, 5% H_2). Here the question is how the oxide, i.e. kind of oxide, overall oxide coverage, island size and distribution, will affect the wettability and the interfacial reaction. For this purpose a novel experimental set-up was designed in cooperation with the group of Dr. Spiegel, comprising thermal treatment and galvanizing units. The wetting is carried out by a sessile drop procedure and can be followed via optical contact angle measurement, and at any desired time the interface can be made accessible for surface analytical investigations by spinning off the excess zinc (liquid) exposing the interfacial reaction layer (solid). The investigations showed that oxide islands can either be overgrown by the Fe_2Al_5 reaction layer or undercut, i.e. they go unto the liquid zinc phase. The latter has been observed for large oxide layers, the first for more realistic oxide islands (100 nm range). One important experimental result is that the overall wetting kinetics is completely governed by this overgrowing of the oxide islands (see Fig. 4, next page).

The main function of zinc coatings is to polarize (by zinc corrosion) defects going down to the steel surface to sufficiently negative potentials so as to prevent corrosion of the steel itself. However, if this were all, significant oxygen reduction would occur at the steel surface polarized to the corrosion potential of zinc, which would need to be fed by increased corrosion of the zinc. An often neglected, but very important, second function of the zinc is that its corrosion products precipitating on the steel surface lead to a significant inhibition of the oxygen

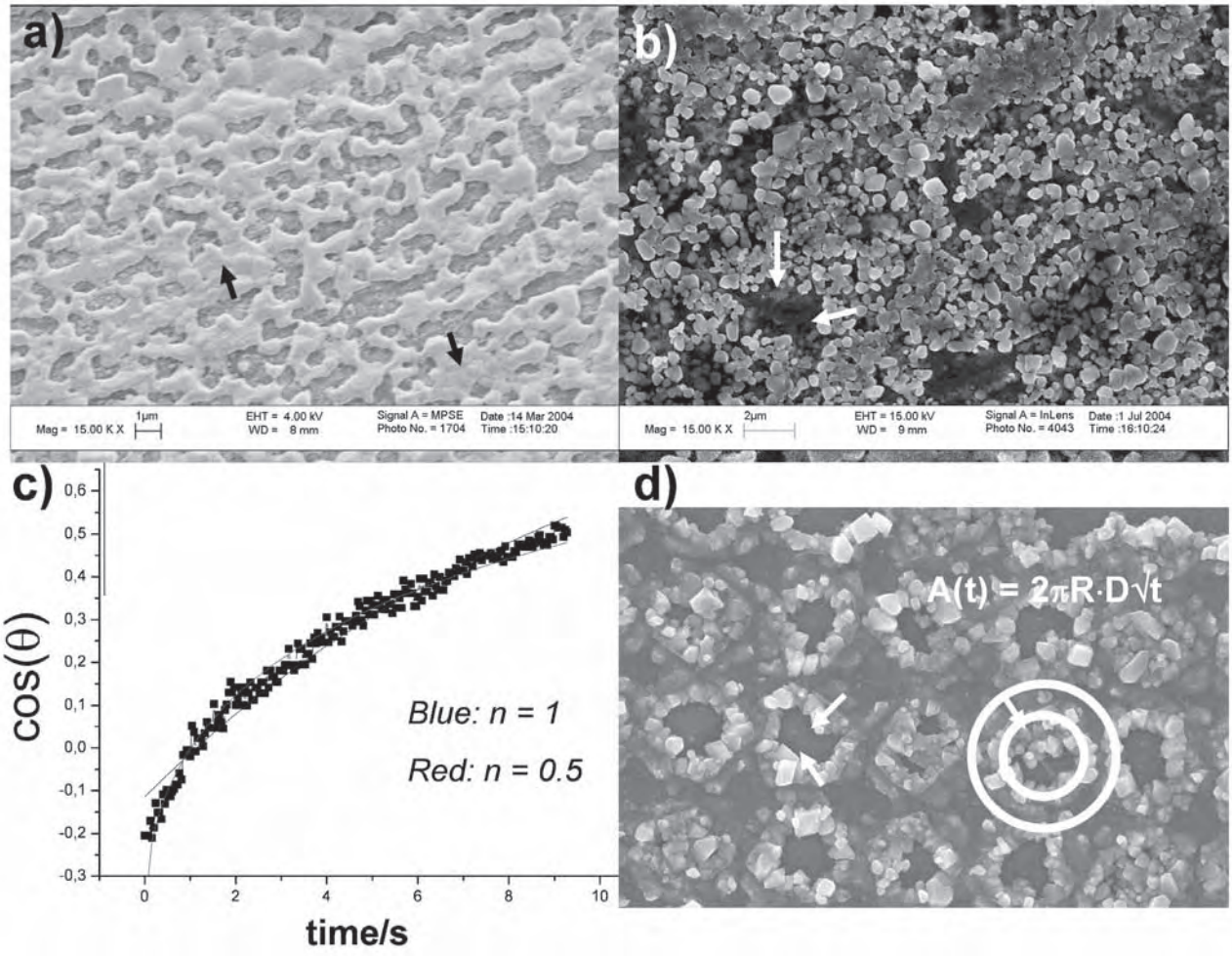

Fig. 4: ***a)*** *SEM image of the oxide coverage (pale grey) on a Fe1.5Si model alloy sample, after simulated industrial annealing and prior to the galvanizing.* ***b)*** *snapshot of the Fe_2Al_5 inhibition layer formation obtained by spinning-off of the liquid zinc after 1s of hot-dip galvanizing.* ***c)*** *contact angle change during wetting (cosθ vs. t); the curve can be fitted by modified Avrami kinetics with an Avrami coefficient of n=0.5 (red curve), although one would expect n=d·0.5=1, as it is the area fraction of the formed inhibition layer that causes the contact angle change, i.e. the dimension d would be expected to be 2. The seemingly one-dimensional character of the growth is assumed to be caused by the outward-inward overgrowth of the inhibition layer, starting at the oxide borders (see arrows), see also the model samples with oxide islands of 2 microns shown in* ***d)****. At least at the initial steps the growth is then determined by more or less one-dimensional growth laws.*

reduction, thusly relieving the corrosion pressure from the zinc coating. This important inhibition of oxygen reduction in the defect is considerably improved by Mg additions. For obtaining a more fundamental understanding of the inhibition mechanisms the effect of alloying elements in the zinc layer is investigated in a dedicated European research project.

2. Self-healing coatings

Another strategy for improved performance is investigated in the same project, namely the storage of inhibitor filled encapsulated mesoporous silica particles in the zinc coating. Only when corrosion occurs the particles will be released and the encapsulation opens at the high pH prevailing at the defect, releasing the inhibitors. One of the main problems in the research project is the co-deposition of the particles with the zinc. In addition, fundamental research on the properties of such silica particles is carried out in cooperation with Dr. F. Marlow of MPIK in Mülheim within the IMPRS-SurMat [31].

Of special interest for such intelligent self-healing are organic composite coatings containing conducting polymer nano-particles. It could be shown for the first time why sometimes coatings reported to provide good corrosion protection disastrously fail under more applied corrosion conditions [17-19], and how coatings should be designed in order to provide a reliable general good corrosion protection [18,20]. This is discussed in more detail in a separate contribution, where it is shown that the research on the fundamental mechanisms of ICPs also provides new and very fundamental insight on the delamination process itself.

3. Fundamental delamination studies and interlinking with simulation groups

This is in direct correlation to the work on basic delamination mechanisms at the polymer/metal interface, which have started with making AFM in the Kelvin mode available for delamination studies [12]. As a next step it is tried to perform fundamental studies on the electrochemistry and delamination behaviour of model samples based on thiol/Au(111) for providing information on the correlation between molecular structure at the interface and degradation mechanisms as input and feedback for simulation work. First results point out that the reactions are preferentially taking place at defect sites such as domain boundaries. Hence, during the initial phase of the project the main input for the simulation will be information on the different kinds of defect sites and on their relevance for the electrochemical processes so as to help focussing the simulation work to the relevant systems (cooperation with Dr. Alexander T. Blumenau). In addition to this work a new project has started where the focus will be on the semiconducting properties of passive oxides, which have been found in the case of $MgZn_2$ to determine the overall delamination process. As a start the effect of oxygen partial pressure will be investigated (in cooperation with Prof. Jörg Neugebauer).

3. Adhesion and Thin Films (PD Dr.-Ing. habil. G. Grundmeier)

Main research areas and vision of the group

The Adhesion and Thin Films group focuses the molecular understanding of adhesion and the tailoring of materials surfaces and interfaces with thin functional films. The main vision is to design functional interface dominated materials such as layered coatings or nanocomposites based on a molecular understanding of the interface structure and stability.

Current topics of the group are:

i. Fundamental aspects of molecular adhesion
ii. Interaction of low pressure and atmospheric cold plasmas with metal and polymer surfaces and tailoring of thin functional plasma polymer films
iii. Structure, functional properties and stability of metal/polymer nanocomposite films
iv. Adhesion and de-adhesion mechanisms of adhesives
v. Design of spectroelectrochemical techniques for the in-situ analysis of polymer/metal interfaces

Recent highlights

Polymer/metal adhesion in humid environments is determined by the resulting molecular forces and the electrochemical reactions occurring at the polymer/metal interface. Very few techniques exist to analyse the transport phenomena of ions and water along polymer/metal interfaces as the dominating process that precedes de-adhesion. Recent studies focused on the design of combined spectroscopic and electrochemical techniques to provide a detailed understanding of the mobility of water and ions along polymer/metal interphases. By means of combined scanning FTIR-ATR-spectroscopy and Scanning Kelvin Probe measurements it became for the first time possible to measure in-situ the transport kinetics of water and hydrated ions along the interphase and interface in polymer/metal composites. E.g. it could be shown that the transport kinetics of water along polymer/metal interphases is two orders of magnitude faster than the bulk diffusion [10,11]. Moreover, the transport of hydrated ions is coupled to the interfacial water transport.

A new in-situ spectroelectrochemical set-up combining electrochemical impedance spectroscopy and FTIR-ATR spectroscopy for the analysis of water uptake and interface chemistry in polymer/oxide/metal interphases was designed. Furthermore, vibrational spectroscopy was applied for the study of the adsorption and adhesion of monomolecular layers by means of Surface Enhanced Raman Spectroscopy [32].

A height regulated Scanning Kelvin Probe (HR-SKP) that is capable of measuring the sample/needle distance and the interfacial electrode potential at the same time has been constructed for the study of rough or curved surfaces in humid environments [32]. Moreover, the height regulation leads to an improvement of the spatial resolution since the distance between the vibrating needle (i.e. the reference electrode) and the substrate surface can be kept to a minimum. The height regulation is performed by a double modulation of the external voltage at different frequencies. The new HR-SKP has been applied to different forms of corrosion including filiform corrosion on organically coated aluminium samples. Moreover, a combination of a pressurized Blister Test and the HR-SKP has been realized that was applied for the study of adhesives under both corrosive and mechanical load.

Tailoring of materials' surfaces and thin films is done in various research projects and new surface modification techniques such as plasma and PVD processes are developed for the deposition of functional films [33,34]. These films can be designed

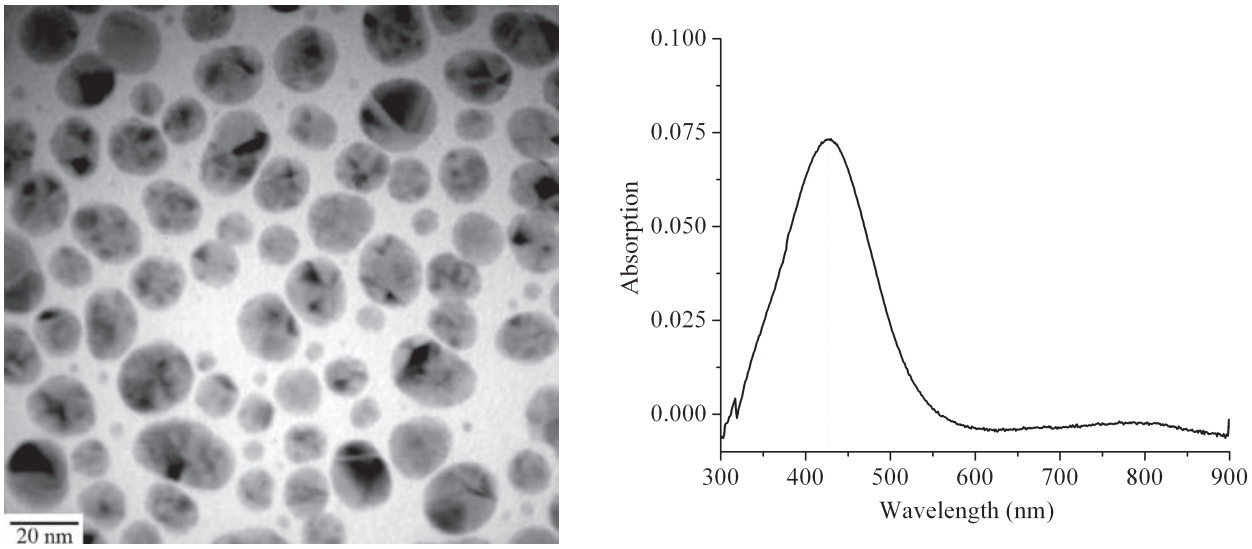

Fig. 5: ***a)*** *TEM analysis of model monolayer nanocomposite films with Ag-nanoparticles included in a perfluorinated plasma polymer matrix,* ***b)*** *Corresponding UV-Vis spectrum revealing the surface plasmon resonance of the embedded Ag-nanoparticles.*

in a manifold manner with respect to chemical composition, morphology, surface energy barrier as well as optical and mechanical properties. Recently, the investigations focused on the understanding of the release mechanisms of Ag-ions from Ag-nanoparticle containing perfluorinated plasma polymer films. The studies provide insight into the stability of the nanosized Ag-particles and the release mechanism.

Cooperative studies

The Adhesion and Thin Film group works in close cooperation with the group of Dr. Blumenau in the field of the theoretical understanding of molecular adhesion phenomena. Scientists who perform complementary experimental and theoretical studies are cooperatively guided. In the field of metal/polymer nanocomposite films the group closely cooperates with the chair of Materials Composites headed by Prof. F. Faupel at the university in Kiel. As part of the scientific programme of the IMPRS-SurMat, SERS studies are done in collaboration with Prof. Tian from Xiamen University and microscopic analysis of metal nanoclusters in polymers as well as molecular adhesion promotion is done in close cooperation with the group of Prof. Eggeler at the university in Bochum.

4. Electrochemistry and Corrosion (Dr. A.W. Hassel)

The vision of the Electrochemistry and Corrosion group is a systematic understanding, adjustment and utilisation of the logical triangle crystallography, passivity and micro- or nanostructure for the development, improvement and shaping of materials (Fig. 6). Crystallography in this sense involves both, the crystallographic structure and the crystallographic orientation of the material. Passivity is understood as a usually desired material property; for electropolishing, electrochemical micromaching or phase selective dissolution however, a phase selective, local or temporal suspension of the passive state is required but has to be kept under strict thermodynamic or kinetic control. Corrosion of materials is frequently a local process and needs investigations in microscopic or even nanoscopic dimensions. The corrosion rate can be quite different for different crystallographic orientations (grains) and especially in the grain boundaries. But also for materials that exhibit the ability for a phase transformation such as shape memory alloys or TRIP / TWIP materials this aspect must be regarded.

Major research areas are:

i. metallic nanodevices
ii. tribocorrosion and chemical mechanical planarization
iii. corrosion of novel materials
iv. combinatorial alloy development

1. Nanotechnology: a link between directional solidification and electrochemistry

Directional solidification of eutectics is a method that is used for the fabrication of large high temperature resistant devices. This method combined with a systematic knowledge based electrochemical treatment allows the production of a number of nanodevices such as nanowire arrays [35], isolated nanowires [36], nanopore arrays [37,38], novel STM tips and so on [39]. This method has been successfully combined with electrodeposition of metals such as gold to prepare ultra micro disc

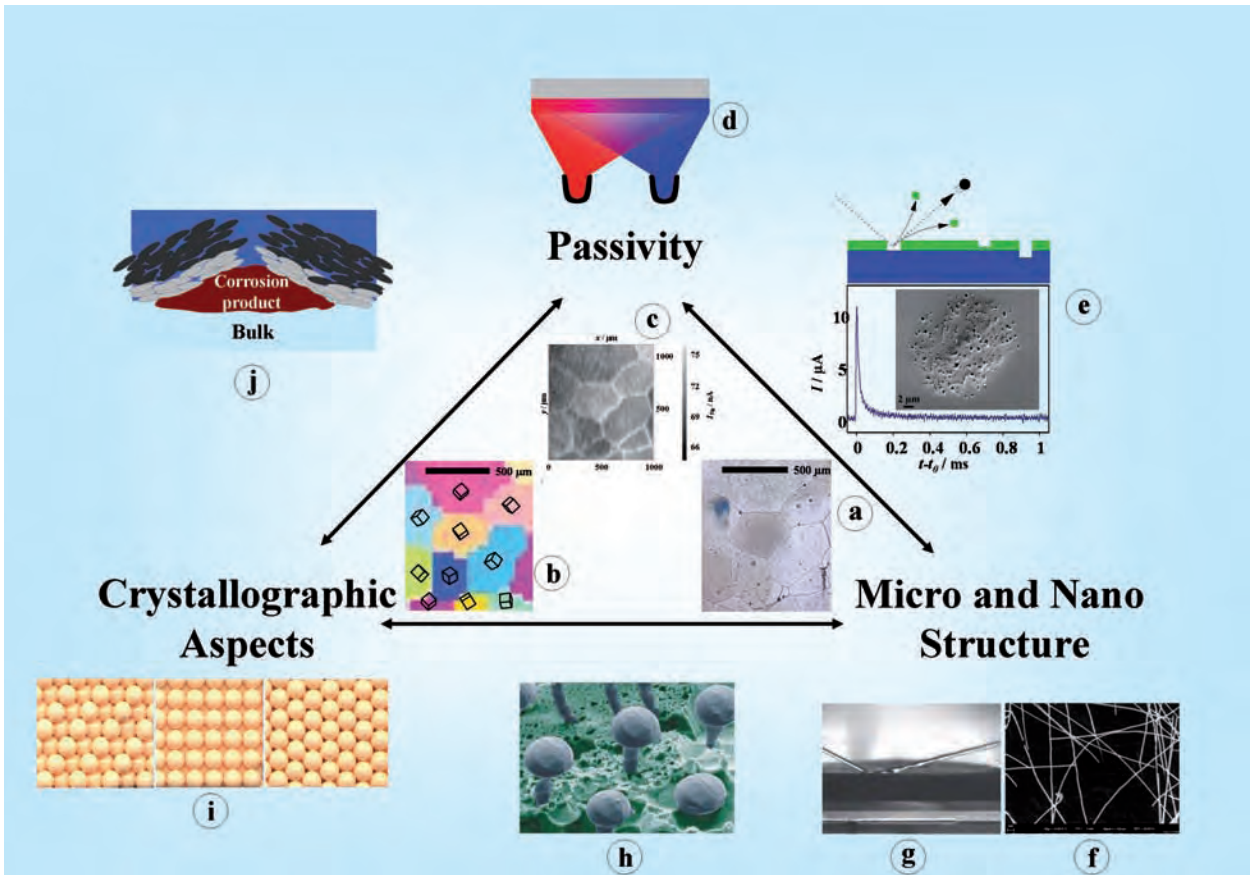

Fig. 6: *The scientific focus of the Electrochemistry and Corrosion group spans between passivity, crystallography and µ/nano-structure of materials.* ***a)*** *the optical image of a light weight ferritic FeAlCr steel shows its grain structure,* ***b)*** *an EBSD map of the same sample reveals the crystallography behind,* ***c)*** *a scanning electrochemical microscopy SECM images directly the reactivity of the sample in the passive state,* ***d)*** *schematic of combinatorial alloy development using codeposition,* ***e)*** *investigation of particle induced flow corrosion by current transients from single particle impacts and resulting impact crater (inset),* ***f)*** *directional solidification (ds) produces W nanowires with aspect ratios > 1000,* ***g)*** *PTFE sputtered nanowire arrays show extreme hydrophobicity, that can even reflect a water jet,* ***h)*** *Re nanollipops are clone like structures with identical morphology,* ***i)*** *crystallographic elementary planes,* ***j)*** *schematic of the final situation in the corrosion of a thermal spray coating.*

electrode arrays [40] and arrays of recessed nano disc electrodes [39] for future applications in sensors. These systems are ideal model systems for studying superhydrophobicity since the surface functionality can be varied from hydrophilic to ultrahydrophobic [41]. The wire diameter and the spacing can be quantitatively described as a function of growth rate and temperature gradient [38,42]. A number of collaborations (R. Adelung, F. Faupel, Kiel; A. Gölzhäuser, Bielefeld; V. Cimalla, Ilmenau; G. Fahsold, Heidelberg; D. Zerulla, Dublin; T. Wübben, Stuttgart) have been established with a vivid exchange of samples, knowledge and share of methods. This research aims at producing nanostructures being applicable at high temperatures of several hundred °C showing quantum confinement under these conditions. A generalized method has been established that allows employing eutectic systems, governing growth factors that control diameter and interfibre spacing [42] and controlling a desired dissolution under either thermodynamic or kinetic control [35-37]. Feasibility studies for the production of nanodevices were successful for nanowires, nanowire arrays as field emitters and novel STM tips.

2. Slurry jet: real time monitoring of a single particle impact and its scientific impact

An experimental setup has been constructed that allows studying single particle impacts in multi-phase flow induced corrosion [43]. It allows studying the effect of particle morphology [44] and a quantitative description of the normal (indent) and lateral (scratch) component during impact under various angles [45]. This method is also useful when studying the chemical mechanical planarization (CMP) in the copper damascene process in semiconductor processing [46] and the adsorption kinetics and protection efficiency of alternative inhibitors [47]. It could be demonstrated that fatty and organic acids, namely sorbate are able to improve the passivation of copper during CMP. By means of the slurry jet it was possible to demonstrate that the commonly used

copper inhibitor benzotriazole adsorbs too slowly for being used in the CMP but sorbate on the other hand is able to extend the passivity range of copper in alkaline solutions by several hundred mV depending on the sorbate concentration.

3. Phase transforming materials: flexibility when needed

NiTi is a shape memory alloy that is attracting a significantly increasing interest for applications such as actors and as implant materials in medical applications. The scientific focus of the group lies on the improvement of surface properties and extension of possible applications by surface engineering of this binary alloy [48]. The mechanism of electropolishing in methanolic sulphuric acid was studied and the best solution was found to be 3 molar in acid with a small amount of water at temperatures below the freezing point of water [3]. In an attempt to further lower the nickel run off from the surface that can be detrimental for medical applications, three different strategies are presently applied. The first is a high voltage anodisation with short voltage pulses of up to 200 V which allow forming a tile structured surface [4]. Oxy chlorination in a properly controlled atmosphere (cooperation with Dr. Spiegel) allows a selective oxidation of titanium and a simultaneous chlorination of the nickel that exhibits significant volatility of the $NiCl_3$ resulting in a strictly Ni depleted titanium oxide film with underlying Ni_3Ti interface [49]. Within the frame of the IMPRS-SurMat a similar approach is made electrochemically now based on a control of the ion concentrations in solution (cooperation with G. Eggeler, RUB Bochum).

4. Combinatorial material development: looking for a needle in a haystack - systematically

A novel approach is made in the development of materials by means of a multi source thermal codeposition unit for the preparation of 2 dimensionally graded materials. This combinatorial alloy development must be combined with an effective high throughput screening by scanning techniques such as scanning droplet cell, scanning Kelvin probe, EDX and Raman microscopy. A recent application is the development of new patina forming steels, so-called weathering steels. They have the ability to develop passivity as a result of accumulated minor elements which can stimulate a phase transformation of the corrosion products resulting in a thick redox-invariant patina. First samples of graded materials were already produced and tested. They allowed an easy assessment of a critical composition for a specific corrosion condition.

5. Atomistic Modelling in Interface Science (Dr. A.T. Blumenau)

This new research group was established in September 2004. It is mainly focused on the following topics:

i. atomistic structure of organic monolayers on metal(oxide) surfaces
ii. adhesion and de-adhesion of organic molecules on surfaces and interfaces
iii. delamination mechanisms at interfaces between metal(oxide)s and organic coatings
iv. atomistic and electronic structure of dislocation cores in semiconducting materials

To achieve a better understanding of these interface related phenomena on the molecular and atomistic scale in more detail than possible by sophisticated experiments only, experiment and theory have to be combined in a process of mutual validation. Therefore the group closely interacts with the department's experimental groups, in order to design new experiments on well defined model systems and structures, which are feasible for computational modelling. This is in particular supported by the preparation of well defined substrate surfaces in the UHV system of the department. *On the other hand, regarding its computational modelling activities, the group is virtually also embedded in the Department of Computational Materials Design with a constant exchange of know-how and furthermore sharing a common computational infrastructure and resources.*

Methodology

The group's theoretical modelling is primarily based on density functional theory (DFT), where the highly complex many-electron wave function is replaced by an overall spatial electron density. With the included approximations for the exchange-correlation-functional, DFT does however fail for specific bonding configurations and is often not sufficient when it comes to describe organo-chemical reactions at surfaces and interfaces. The application of less approximate but computationally more demanding *ab initio* methods then becomes inevitable. However, as the modelling of larger molecules on surfaces and of organic/inorganic interfaces requires atomistic models of hundreds of atoms, such methods cannot be applied easily. Nevertheless the group abandoned the common DFT-only approach and – as a first step towards a multiscale combination of methods – now includes wave function methods beyond DFT on small model systems as a reference and validation for the DFT calculations made to extrapolate to larger systems.

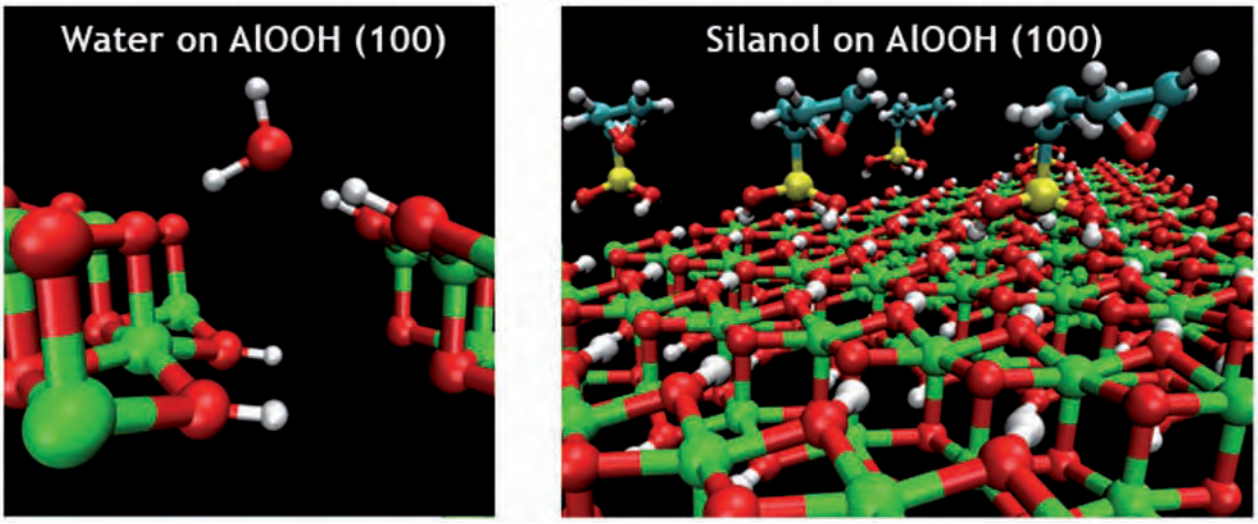

Fig. 7: *Simulation snapshots of the adsorption of water (left) and of a Silanol monolayer (right) on a hydroxide layer.*

Hence by the group's approach, which extends beyond DFT into the field of computationally very demanding *ab initio* wave function methods, the modelling of organic molecules on surfaces and at interfaces is put on a broader and more reliable basis than usually done and a common source of error is considerably reduced. This allows a predictive modelling, which can help to interpret and understand experiments on an atomistic or molecular level and additionally guide and inspire new experiments.

Activities of the group

The methods described above are applied to a variety of technologically relevant interface problems. The following three examples illustrate the general directions of the group's research.

1. Fundamental delamination studies

Understanding and controlling polymer delamination at polymer/metal interfaces is a challenge of great technological relevance as it promotes corrosion of the underlying metal. To understand the involved fundamental electrochemical processes, a combined approach of theoretical modelling and experimental techniques appears most promising. Therefore thiol molecules on gold are chosen as a model system to study the elementary processes such as ion diffusion along the interface, oxygen reduction and film degradation through radicals – all in close collaboration with the Molecular Structure and Surface Modification group of Dr. Michael Rohwerder. A very important ingredient in the studies is the atomistic structure of the interface, and in particular the thiol's binding sites on the surface – which remains a disputed topic. The group was able to identify two possible distinct binding sites for methyl thiol on Au(111), where the molecule is tilted in opposing directions. These two possible sites combined with the 3 equivalent directions on the surface already for methyl thiol give 6 different domains for self assembled monolayers. In parallel, the mechanism of oxygen reduction, which is believed to be a key process in the delamination and degradation process of the organic film, is investigated including the effect of water as a solvent via a self-consistent-isodensity polarisable continuum model.

In the course of this work various DFT functionals and wave function based-methods have been compared with each other in a test set for different basis sets in order to estimate their accuracy and deviations. This accuracy map allows to estimate the error bars of the current and future calculations on SAM degradation on gold.

2. Adhesion on oxide films

Besides the delamination studies mentioned above, which are focused on a pure model system and aim at understanding fundamental mechanisms, the group together with the Christian Doppler Laboratory and Dr. Guido Grundmeier investigates molecular adhesion on technologically relevant aluminium oxides and zinc oxides. Fig. 7 shows a monolayer of an organic bonding agent as used in adhesion chemistry on aluminium oxyhydroxide. Such model systems serve as first investigations of polymers or primers attached directly to a metal oxide ("direct bonding"). Direct bonding mechanisms might play an important role in the industrial surface treatment of steel sheets. Further, the competition between the bonding of organic molecules to the oxide and the bonding of water molecules to the oxide is investigated.

In a first step, water and silanol adsorption on the (001)-surface of boehmite has been considered. On an amorphous – or better nano-polycrystalline –

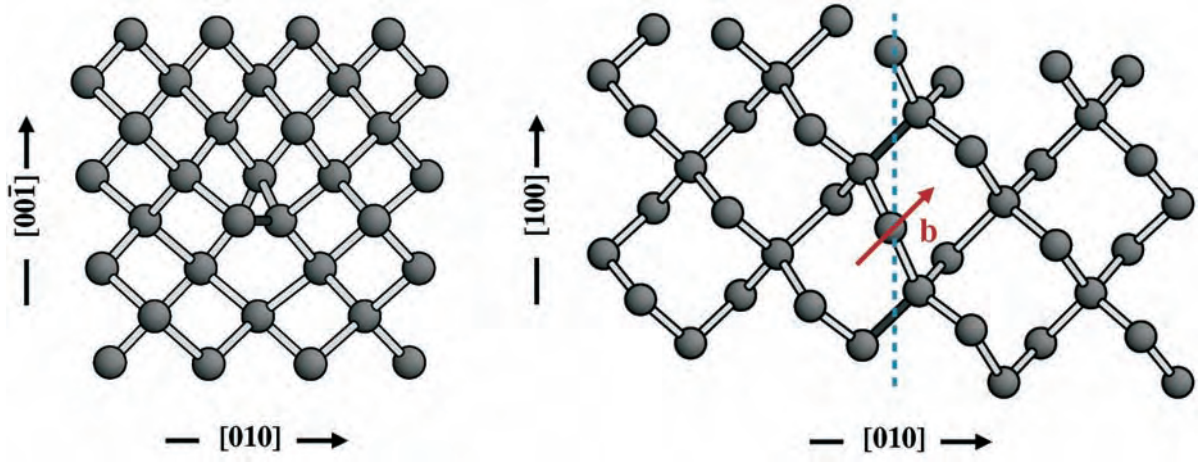

Fig. 8: *Cross sectional view of the low energy core structure of the <100> mixed type dislocation in diamond (left) and a view onto the glide plane of the same structure (right).*

surface, we can expect that 20-24 % of the boehmite surface sample are (001) oriented (P. Raybaud, et al., J. Cat. 201 (2001) 236). In DFT plane wave pseudopotential calculations both water and silanol adsorption appear to be driven by weak hydrogen bonding. As no change in oxygen hybridisation occurs, no covalent/ionic bonds can form. For mainly geometrical reasons bonding appears to be stronger when only two of the three OH groups are involved. Next steps will include the investigation of further surface orientations and different types of silanol molecules. The improved molecular understanding of the bonding mechanism and the corresponding adhesion strength will allow to identify optimum requirements regarding the chemical composition and structure of the oxide film and regarding the functionality of the involved organic molecules.

3. Dislocation cores in semiconducting materials

Recent advances in the growth of high quality single crystal CVD diamond have led to an increased interest in <100> dislocations. These dislocations are observed as mixed-type 45° and pure edge dislocations, however their atomistic core structure and their possible detrimental influence on the electronic properties is still unclear. Hence DFT and DFT-based methods are used to predict the atomistic and electronic structure of the dislocation cores. Furthermore, in an approach combining atomistic modelling with elasticity theory, the dislocation core energies are determined. However, unlike the usual and widespread approach, which is based on empirical potentials only, here the underlying atomistic method is fully based on DFT in order to correctly describe the covalent reconstruction bonds in the core and to allow investigating relative stabilities of the core structures. It is found that both dislocation types lead to states in the electronic band gap and alternative zigzagged core structures could be ruled out as being by far less stable than the straight dislocations [50]. Fig. 8 gives an example of a dislocation core structure in diamond. These results give insight into the effect of non-negligible dislocation densities on future semiconductor devices based on diamond.

As opposed to diamond, the development of devices based on silicon carbide is much more advanced. However, in *pin* diodes, stacking faults are known to expand under forward bias, causing an irreversible degradation of the devices. To understand – and maybe prohibit – this expansion of the faults and hence to stop the degradation, requires understanding the motion of their bordering partial dislocations, which are believed to move via a mechanism of recombination enhanced dislocation glide (REDG). In order to describe this phenomenon, the migration of kinks at the dislocation lines has been modelled with respect to the effects of charge accumulation at the dislocation line [51,52], suggesting possible REDG mechanisms.

Work on the field of dislocations is done in collaboration with N. Fujita, T.A.G. Eberlein and R. Jones at the University of Exeter (UK) and with S. Öberg, Department of Mathematics, Luleå University of Technology, Sweden.

Future

The group plans to continue the work described above. Regarding adhesion on oxide films, links to experiments will be established by modelling experimentally accessible spectra (e.g. infrared) and by comparing binding energies with thermodesorption spectroscopy. Furthermore single molecule adhesion will be studied both experimentally and theoretically to get a more fundamental understanding of adhesion on.

Studies of delamination and degradation of organic films on metals will be broadened, including modelling

more demanding processes such as ion and water diffusion along the interface and the destruction of the organic coating by radicals formed during cathodic delamination and corrosion. As the chosen model system (thiol SAMs on gold) plays an important role also in the field of metallic nanoparticles functionalised by organic chemistry, the group will further expand its activities into this direction.

Outlook

After 6 years the Department of Interface Chemistry and Surface Engineering has a well established organization, is internationally highly visible and has strong links to the German and international steel industry. The department is internationally leading in the area of steel surface technology and hosts many large international projects with scientific and industrial groups.

The foreseeable future is determined by the following developments:

(1) The group "Adhesion and Thin Films" of PD Dr. Guido Grundmeier will not be continued in the long run, as Dr. Grundmeier accepted an offer as Full Professor and head of the chair for "Technical and Macromolecular Chemistry" at the University of Paderborn. The loss of this group, which is one of largest of the institute, will require major rearrangements of the department. Some subjects which in the past have been investigated by this group will be taken over by other groups in order to reduce scientific overlap. A new group will have to be established probably with a strong focus in polymer science and (non-linear) optical spectroscopy. The area of adhesion science will continue to be very important in the department.

(2) Research aiming at an atomistic or molecular understanding of reactions on surfaces and at interfaces will be strengthened. This includes typical surface science approaches but also a further strengthening of studies providing information of molecular interactions at interfaces. It is expected that in-situ synchrotron based experiments in close collaboration with Anke Pyzalla will also gain importance.

(3) Theory will gain importance, too. It I a clear aim to link experiment and theory as much as possible and to further strengthen the theory group in the department as well as the collaboration with Jörg Neugebauer. The department has been leading in the establishment of a new theory department for Materials Science at the Ruhr-Universität Bochum (**I**nterdisciplinary **C**entre for **A**dvanced **M**aterials **S**imulation, ICAMS) sponsored by German materials industry. It is expected, that subjects like interface engineering will be of prime interest for this new department and the group of Dr. Blumenau will have very close ties to this new centre.

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Research Projects in Progress

Adhesion and Thin Films

Giza, Grundmeier: Plasma modification of oxides on seminconductors and metals

Titz, Grundmeier: Structure and properties of corrosion resistant thin plasma polymer films on zinc coated steel sheet

Thissen, Grundmeier: Self-assembled adhesion promoting monolayers on plasma modified oxides

Wang, Grundmeier: Plasma polymer/metal nanocomposite films

Sun, Grundmeier: Application of SERS to the adhesion and de-adhesion of thin organic films

Valtiner, Grundmeier: Single Molecule Adhesion on Zn-oxide single crystals

Popova, Grundmeier: Chemical Force Microscopy on oxide covered metals in corrosive environments

Fink, Grundmeier: Analysis of thin hybrid conversion films on galvanised steel sheet

Klimow, Grundmeier: Application of the Scanning Kelvin Probe Blister Test for adhesion studies

Lehtinen, Blumenau, Grundmeier: DFT analysis of the structure and the adhesive properties of Al-oxy-hydroxides

Vlasak, Grundmeier: Spectroelectrochemical studies of polymer/metal interphases

Özcan, Blumenau, Grundmeier: DFT analysis of the adsorption and adhesion of silanols on Zn-oxide single crystals

Posner, Grundmeier: SKP studies of the mobility of hydrated ions in polymeric interphases

Wapner, Grundmeier: Interfacial barrier properties of dispersion coatings with different glass transition temperatures

Zuo, Grundmeier: Analysis of Ag nanoclusters in TiO_2-matrix for photochromic applications

Keil, Grundmeier: Application of NEXAFS to the analysis of metal/polymer nanocomposite films

Itani, Grundmeier: Synthesis and analysis of metal nanoclusters in polyelectrolyte thin films

Atomistic Modelling in Interface Science

Biedermann, Blumenau: Numerical modelling / lifetime prediction of delamination polymer coating disbonding and material degradation (Thiol SAMs on Au)

Torres, Biedermann, Blumenau: Numerical modelling of Thiol SAMs on Au

Lehtinen, Blumenau, Grundmeier: DFT analysis of the structure and the adhesive properties of Al-oxy-hydroxides

Özcan, Blumenau, Grundmeier: DFT analysis of the adsorption and adhesion of silanols on Zn-oxide single crystals

Fujita (Exeter), Blumenau: Modelling dislocation cores and core-impurity interaction in semiconducting materials (collaboration N. Fujita, T.A.G. Eberlein and R. Jones (Exeter, UK) and S. Öberg (Luleå, Sweden))

Electrochemistry and Corrosion

Smith, Akiyama, Hassel: Detection of discrete and single impacts in particle induced flow corrosion

Bello Rodriguez, Milenkovic, Schneider, Hassel: Production of nanowire arrays through directional solidification and their application

Bruder, Hassel: New approaches in electrolytic cleaning of cold rolled steel sheets

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

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

Fushimi, Hassel: Electropolishing of Nitinol based shape memory alloys

Lill, Hassel, Sauerhammer, Spiegel: Corrosion and corrosion protection of TRIP/TWIP steels

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

Mingers, Hassel: Delamination of thermal spray coatings

Mozalev, Poznyak, Hassel: Nanostructured aluminium tantalum composite oxides

Tan, Hassel: Design and Construction of a sub-micron indenter for tribological investigations

Yadav, Manthey, Hassel: High throughput screening of corrosion behaviour in combinatorial alloy development of patina forming steels

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

Brittman, Smith, Hassel: Selective electrochemical dissolution of a directionally solidified Ag-Cu eutectic

Perezim, Milenkovic, Hassel, Crystal growth in an induction field with gradient

Chen, Tian, Hassel: Random versus organised one dimensional gold nanoparticles and their spectroscopic characterisation

Hassel, Ek: Metal corrosion in contact with clay

Luty, Milenkovic, Hassel: Directional solidification and microstructural investigations of Al-Bi monotectic alloys

Fenster, Rohwerder, Hassel: Reactivity of zinc and novel zinc alloys under pH, CO and CO_2 influence monitored by impedance titration

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

Dönecke, Lill, Rablbauer, Hassel: Corrosion of ferritic FeAlCr light weight steels

Bello Rodriguez, Smith, Milenkovic, Hassel: Application of Directionally Solidified Nanowire Arrays

High-Temperature Reactions

Asteman, Spiegel: Materials for increased performance in sustainable fuel combustion

Asteman, Lill, Hassel, Spiegel: Semiconducting properties of high temperature model oxides

Asteman, Spiegel: Mechanisms of alumina scale growth at low temperatures

Hüning, Borodin, Rohwerder, Spiegel: Initial stages of oxidation of Fe-Cr alloys

Liapina, Spiegel: Initial stages and kinetics of oxidation of binary and ternary iron-aluminides

Mardare, Spiegel: Spinel oxide coatings on steels for SOFC application

Parezanovic, Spiegel: Oxidation and segregation on high strength steels

Ruh, Spiegel: Optimisation of in-service performance of boiler steels by modelling high temperature corrosion OPTICORR

Sanchez-Pasten, Spiegel: Investigations on the high temperature corrosion of metallic materials under waste incineration conditions at temperatures of 300 to 600 °C

Schmitt, Vogel.D, Spiegel: Simulation of heat and gas flow in high temperature microbalance

Srinivasan, Spiegel: Microscopic aspects of alloy oxidation

Vogel.A, Spiegel: Mechanistic studies on HCl induced corrosion of carbon steels

Vogel.D, Spiegel: Failure analysis of a Lepol-grid from a cement kiln plant

Vogel.D, Spiegel: Investigation on the oxidation resistance of a diesel engine particle filter

Molecular Structure and Surface Modification

Laaboudi, Rohwerder: Correlation between molecular structure and degradation behaviour for thiol monolayer films on gold as a model system for delamination at polymer/metal interfaces (in cooperation with Dr. Blumenau within a STREP)

Isik-Uppenkamp, Rohwerder: Intelligent corrosion protection based on conducting polymers

Turcu, Rohwerder: Intelligent corrosion protection by nanocapsules incorporated to the zinc coating: self-healing at the cut-edge.

Stempniewicz, Marlow (MPIK), Rohwerder: Release from Mesoporous Silica: Cross-Wall Transport and External Diffusion Barrier

Lyapin, Rohwerder: Fundamental aspects of corrosion and delamination behaviour of novel zinc alloy coatings

Fenster, Hassel, Rohwerder: Photoelectrochem. Investigation of oxygen reduction on zinc alloys

Borissov, Rohwerder: Fundamental investigations on the wetting and interfacial reaction behaviour at the interface liquid zinc/steel (in cooperation with M. Spiegel)

Ankah, Hüning, Rohwerder: Combined EC-STM and TEM investigation of the de-alloying behaviour of copper-gold intermetallic phases.

Borodin, Rohwerder: MBE-based preparation of samples with well characterizable oxide surface layers as model systems for the study of surface modification and delamination

De la Fuente, Rohwerder: Fundamental investigation on the critical salt contamination threshold for the break-down of long-term stability at coating/metal interfaces

Zhong, Rohwerder: On the possible effect of inorganic nanoparticle additions on the corrosion protection performance of organic coatings

Department of Material Diagnostics and Steel Technology

A.R. Pyzalla

Introduction

Being a scientific member of the MPIE since November 1st, 2005, Anke Pyzalla and three of her PhD students moved from TU Wien to MPI für Eisenforschung GmbH, Düsseldorf, on 2nd of January 2006. In the following five months all but two PhD students of Anke Pyzalla's former group have joined the MPIE. In April 2006, Dr. Haroldo Pinto became the group leader "Material Testing" in the department. His focus is on residual stress analyses and mechanical testing. In March 2006, Dr. Aleksander Kostka, who had been a Post-Doc in the Institute of Materials at Ruhr-Universität Bochum, joined the department as group leader for "Microstructure Characterization". He specializes in transmission electron microscopy, in particular in the analyses of defect structures and strain analyses by convergent beam electron diffraction.

Left: View along the 1st floor in hall 9 with new seminar room and offices on the right-hand side; right: renovated staircase in hall 9 (Photos: O. Schoplick, Düsseldorf).

Starting work in temporarily assigned offices, the department could move already in May 2006 in the newly renovated and furnished offices in hall 9. Three laboratories for mechanical testing are currently renovated and furnished, and the main floor space in hall 9 is supposed to be adapted for larger scale material testing equipment latest by December 2007. The photos above and below give an impression of the renovated hall. The X-ray laboratories in the main building of the institute currently are substantially renewed by installing state of the art X-ray diffractometers for phase, texture and residual stress analyses using e.g. the old X-ray generators and platforms available, but, mounting new optics, translation/rotation systems (e.g. Eulerian cradles) and fitting them with modern safety shielding.

Views from the 1st floor into the still nearly empty hall 9 (left) and from the outside on the completely renovated office building with the hall behind (right) (Photos: O. Schoplick, Düsseldorf).

Scientific Concepts

Future work in the department 'Material Diagnostics and Steel Metallurgy' will focus on

1.) *Basic research into microstructure and properties of joints between steels and light metals*
2.) *Characterization of microstructure changes and identification of the elementary processes of wear of steels and hard metals*
3.) *Development of new methods for material characterisation/diagnostics using X-rays, synchrotron X-radiation and neutrons*
4.) *Development of new steels and hard metals using conventional and powder metallurgy*

Medium time objectives in these research areas are:

1.) *Basic research into microstructure and properties of joints between steels and light metals:*
- Understanding formation and growth of intermetallic phases in steel/Al-alloy joints based on experiments, thermodynamic calculations and modelling of diffusion processes
- Determination of mechanical properties of the intermetallic phases and their influence on the mechanical properties of steel/Al-joints
- Deduction of a model describing the formation and growth of intermetallic phases in steel/Al joints
- Development of filler materials based on the model for phase formation and growth and considering the mechanical properties of the phases and the welds
- Manufacturing demonstrators of steel/Al joints with optimised microstructure and properties

→ Development of strategies for joining steels to other dissimilar materials such as e.g. Al-, Ti- and Mg-alloys

2.) *Characterization of microstructure changes and identification of the elementary processes of wear of steels and hard metals*
- Identification of the mechanisms relevant for the formation of strongly deformed nanocrystalline and amorphous layers on worn steel/hard metal surfaces and their dependence on the tribosystem (e.g. wear mechanism, medium)
- Determination of stress/residual stress distributions and their influence on the wear resistance of the first and second body in tribosystems
- Deduction of a model for stress/residual stress formation and relaxation in dependence on wear mechanisms and characteristics of the tribosystem

→ Development of strategies for optimising the microstructure and residual stress state of wear parts, e.g. cutting tools

3.) *Development of new methods for material characterization/diagnostics using X-rays, synchrotron X-radiation and neutrons:*
- Further development of the combined diffraction+tomography technique for investigating damage and failure processes in materials under complex loading conditions. The focus will be on the in-situ determination of damage evolution creep e.g. of ferritic and austenitic steels.
- Development of new methods and sample environment for in-situ characterization of stress formation/relaxation and material behaviour under complex loading conditions e.g. during high temperature oxidation and wear processes. Based on these methods and instrument developments, in co-operation with the department 'Interface Chemistry and Surface Engineering', the development and relaxation of stresses in oxide layers will be investigated in-situ using synchrotron radiation, aiming at the deduction of models describing growth stresses in oxide layers.
- Development of methods for characterizing the intragranular strain/stress distribution in individual crystallites of polycrystalline materials. These methods will be used e.g. for determining the influence of grain boundaries in polycrystalline materials on their strain/stress state under loading, starting with experiments and modelling of strain/stress development in deformed bicrystals in cooperation with the department 'Microstructure Physics and Metal Forming'.

→ Development of methods and instruments for characterizing material and component behaviour in-situ under complex and realistic loading conditions using diffraction, scattering and tomography

4.) *Development of new steels and hard metals using conventional and powder metallurgy :*
- Development of wear-resistant Fe-base steel MMCs by hot extrusion
- Development of nitrided hard materials for cutting applications
- Optimisation of creep resistant steels based on the in-situ synchrotron tomography investigations of void formation and failure

→ Development of new steels and hard metals based on microstructure optimisation, and the results of modelling thermodynamics and kinetics in multi-component systems

Scientific Groups

Most PhD students in the department 'Material Diagnostics and Steel Technology' had already started their projects before moving to the MPI für Eisenforschung; in order not to cause further delay in their thesis work they went on pursuing the thesis work defined at TU Wien.

The organisation concept of the department aims at a matrix structure. The scientific topics outlined above are supposed to be covered by 5 groups specialising in different experimental respectively numerical methods:

a) *Microstructure Characterization*
Group leader: Dr. Aleksander Kostka
Methods: Electron microscopy, in particular TEM

b) *Material Properties and Residual Stresses*
Group leader: Dr.-Ing. Haroldo Cavalcanti Pinto
Methods: Mechanical testing, X-ray residual stress analyses

c) *Material Science using Synchrotron Radiation and Neutrons*
Group leader: N.N.
Methods: Diffraction, scattering and tomography

d) *Engineering Thermodynamics and Kinetics in Multi-Component Systems*
Group leader: N.N.
Methods: Thermodynamic calculations of phase diagrams, modelling of diffusion processes, experimental validation of the models

e) *Metallurgy*
Group leader: N.N.
Methods: Conventional and powder metallurgy

Depending on the research topic and the relevance of the different experimental and/or numerical methods, in future research projects and thesis work will be supervised by two group leaders, a supervisor and a co-supervisor.

Outlook

A new group leader in metallurgy has signed a contract and will start in February 2007. His background is in designing and testing wear resistant Fe-based materials and he will expand the existing metallurgy laboratories by powder metallurgy. His anticipated scientific field is design of new steels manufactured both by conventional and powder metallurgy. He will be in charge of the service group metallurgy.

Search is ongoing for the two further open positions for group leaders, an announcement for a group leader in the field of 'material science with synchrotron radiation and neutrons' will be posted latest in January 2007.

In 2007/2008 the installation of microscopy laboratories in particular with a new analytical TEM is planned in direct neighbourhood to the existing microscopy laboratories of the department 'Microstructure Physics and Metal Forming'.

Research Projects in Progress

Dissimilar Welds

Coelho, Kostka, Pinto, Kocak (GKSS) : Microstructure and residual stresses of dissimilar Mg-alloy welds

Pinto: Microstructure and residual stresses of induction pre-heated laser steel welds

Jank (TU Wien), Kostka: Microstructure and properties of resistance welded steel-Al joints

Agudo, Kostka, Pinto: Aluminium-rich Fe_xAl_y intermetallic phases in steel/Al joints

Characterization of Microstructure Changes and Identification of the Elementary Processes of Wear of Metallic Materials

Barbatti, Garcia (Boehlerit): Wear induced changes of residual stresses in coatings on hard metal tools

Barbatti, di Prinzio (UTC Venezuela), *Garcia* (Boehlerit): Influence of shot peening on residual stresses of alumina coatings and on tool life

New Methods for Material Characterization / Diagnostics using X-rays, Synchrotron X-radiation and Neutrons

Dziecol, Souza: Development of experimental and data evaluation methods for white synchrotron radiation tomography

Isaac, Sauthoff: Method developments for quantifying creep damage evolution using synchrotron radiation tomography

Sket, Barbatti, Sauthoff: 3D synchrotron radiation tomography studies and TEM studies of creep damage evolution in steels

Moscicki, Pinto: Development of a method for determining residual stresses in individual crystallites of a polycrystalline materials using high energy synchrotron radiation

Juricic, Pinto, Kostka: Microstructure, texture and residual stress formation in oxide layers on single and polycrystalline iron

Brito, Pinto, Spiegel: Residual stress formation in oxide layers of FeAl intermetallics

Silva, Pinto, Kostka, Clemens (MU Leoben): Microstructure and residual stresses in oxide layers on high Nb-containing TiAl intermetallics (co-operation with Prof. Dr. H. Clemens, Montan-Universität Leoben, Austria)

Development of New Steels and Hard Metals using Conventional and Powder Metallurgy

Barbatti, Garcia (Boehlerit): Microstructure and properties of nitrided hardmetals

Zaree (TU Wien), Pinto, Reimers (TU Berlin), *Theisen* (RUB): Microstructure and properties of hot extruded wear resistant Steel-MMCs

Pinto, Berns (RUB)*:* Influence of texture on distortion during steel heat treatments

Others

Pinto, Fabritius: Residual stresses in lobster exoskeletons

Department of Materials Technology

G. Frommeyer

Scientific Concepts

The research activities in the Department of Materials Technology are focused on the synthesis and characterization of a variety of novel structural and functional materials. These are iron-based alloys, such as high-strength and supraductile light-weight steels, very fine-grained superplastic high carbon steels and ultrahigh strength pearlitic steels, as well as ordered iron-, nickel-, and titanium aluminides, and high melting point Laves phases. These ordered alloys reveal great potential for high-temperature applications, which demand high warm strength, superior creep, and excellent oxidation resistance. The functional materials with specific physical properties like soft magnetic iron-silicon/aluminum transformer steels and rapidly solidified amorphous iron/cobalt-boron-silicon electromagnetic sensor materials are processed by rapid solidification technologies such as in-rotating-liquid spinning (INROLISP) and planar flow casting meltspinning (PFC) using laboratory facilities of the department. Another centre core of scientific and technological research is the analysis and optimization of process parameters by modeling of continuous casting and rapid solidification in laser welding processes in cooperation with industrial partners.

The following major subjects represent the focal points of the fundamentally and technologically oriented research topics:

- Innovative Steel Research
- Rapid Solidification Technology
- Nanoscopic Characterization of New Materials
- Ordered Alloys for High-Temperature Applications

R. Rablbauer, head of the Innovative Steel Research group, and G. Frommeyer are forcing the development of new steels in strong cooperation with the national steel industry. The quantitative characterization of microstructure and properties of new high-strength steels with excellent formability is based on modern design concepts of transportation systems and principles of physical metallurgy. The governing deformation and work hardening mechanisms of the newly developed steels are Twinning Induced Plasticity (TWIP effect), martensitic Transformation Induced Plasticity (TRIP effect), and Shear Band Induced Plasticity (SIP effect). The steels under investigations are of great importance for engineering applications and are of considerable interest of the German steel industry and worldwide. New projects will be performed in cooperation with the newly established department of Materials Diagnostic and Steel Technology.

The research group Rapid Solidification Technology, headed by J. Gnauk, has also a strong relation to the ongoing activities in the steel technology development because this group deals with modeling of casting process technology, to refine existing and produce new superior material properties, guided by intense numerical simulations of the solidification process.

The physical and mechanical properties as well as the chemical and corrosion resistance of steels and other materials are controlled by their microstructures and lattice defects on the atomic scale. For this purpose the department operates an analytical TEM (transmission electron microscope equiped with EDS) and an APFIM facility (atom probe field ion microscope). The results of these investigations on different alloys and research topics are represented in the section Nanoscopic Characterization of New Materials.

Microstructures, mechanical properties, and structural superplasticity of high carbon-aluminium steels and ultrafine-grained aluminides of the transition metals, such as $Fe_3Al(Cr)$, NiAl(Cr) and TiAl(Cr,Mo,Cu) alloys have been extensively studied in recent years. The main objectives are the quantitative description of the microstructure related superplastic deformation and accommodation mechanisms.

Modern steel development is based on the constitution of multiphase iron alloys providing necessary knowledge about thermodynamic and kinetics of phase transformations. These research activities, which were a basic topic of the former Department of Physical Metallurgy performed by G. Inden and G. Sauthoff, have been integrated into the department by the ongoing research of F. Stein and M. Palm. The work is related to the determination of complex ternary phase diagrams based on iron and other transition metals and ordered phases of scientific and technical interest.

Innovative Steel Research

Advanced design concepts of transportation systems, mechanical engineering constructions and architecture structures require high strength steels with high elastic stiffness, excellent formability, superior fractures toughness, and reduced specific weight.

The important aims of innovative steel research rely on the great challenges of steels with superior properties because of the strong competition with the light-weight metals aluminium, magnesium or polymer-based composites. Other important aspects are environmental requirements like reduced exhaust CO_2 and NO_x gases and savings of minerals, oil and natural gas resources. In the last few years new classes of high manganese steels, such as TWIP, m-TRIP and TRIPLEX steel have been developed in the department and are now the subjects of industrial upscaling and implementation for a wide range of industrial applications. The different fundamental deformation mechanisms and typical microstructures of these steels are illustrated in Fig. 1.

High-manganese austenitic steels containing 15 to 25 mass% Mn and additions of silicon and aluminum of about 2 to 4 mass% exhibit high strength and exceptional plasticity due to extensive twin formation under mechanical load (TWIP effect: Twinning Induced Plasticity) or via multiple martensitic transformations (TRIP effect: Transformation Induced Plasticity) [1]. An essential property of deep drawing steels for automotive bodies and frame structures is the impact behaviour. Temperature dependent Charpy V-notch impact tests revealed high energy absorption and that the TWIP steels behave completely ductile, even at very low temperatures of -196 °C [2].

The TRIP-/TWIP-effect of Al and Si alloyed Mn-steels can be successfully expanded to high carbon containing steel grades where Mn is partly substituted by C. High tensile strength and uniform elongations are achieved by increasing the carbon content of these alloys to a certain extend in combination with an excellent deep drawing ability [3].

In the last two years the steel research activity was focused on the design of new super TRIP steels exhibiting a high flow stress of about 1400 MPa and ultimate tensile strength of 1740 MPa, respectively, with relatively high elongation to failure of ε_{pl} = 37 %.

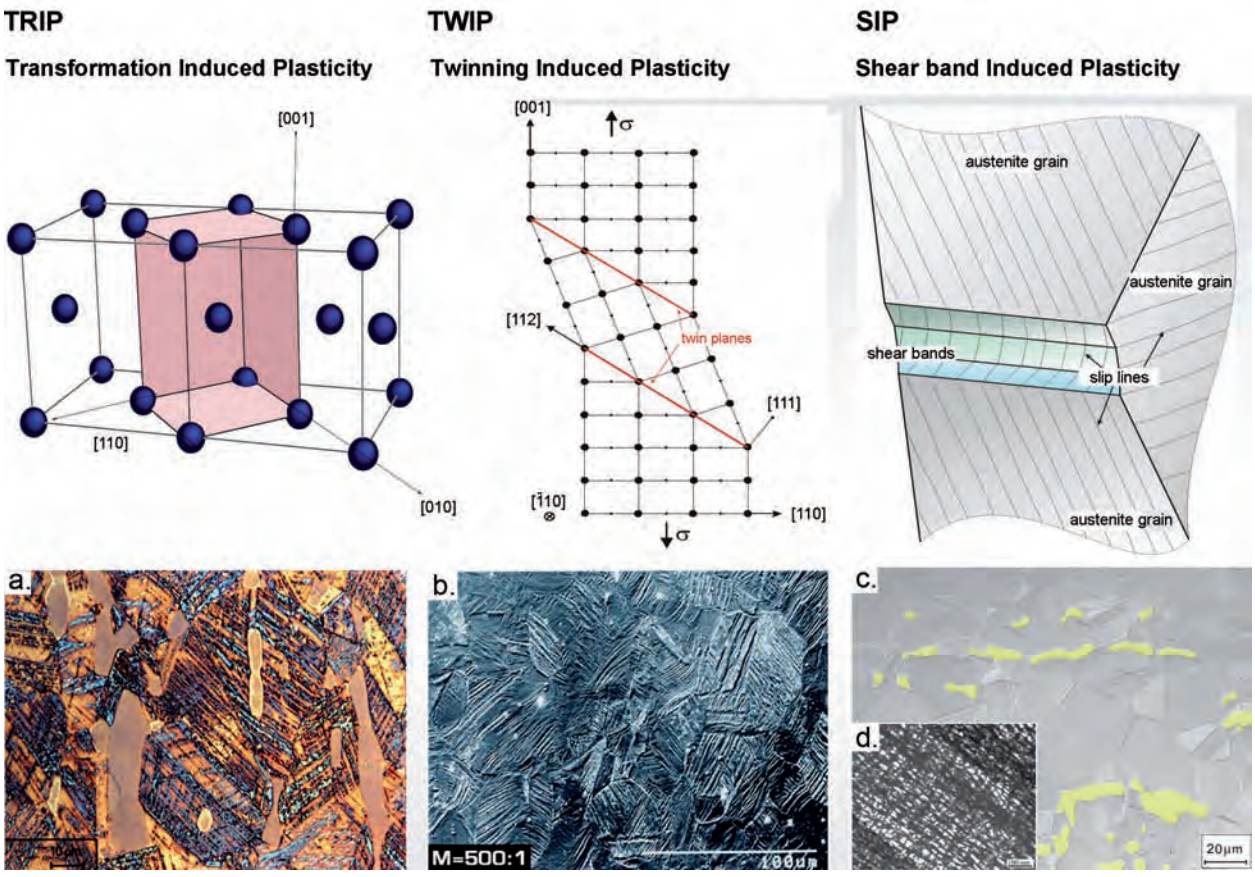

Fig. 1: *Schematic drawings of the governing transformation mechanisms and the resulting microstructural features of different high manganese austenitic steel grades in the as cold deformed state. The optical micrograph of the etched surface demonstrates multiple α_{bcc} and ε_{hcp} martensite transformation in TRIP steel (a). SEM image of TWIP steel showing a high density of deformation twins (b). TRIPLEX steel contains ferrite (yellow) (c) and finely dispersed κ-carbides revealed by TEM (d).*

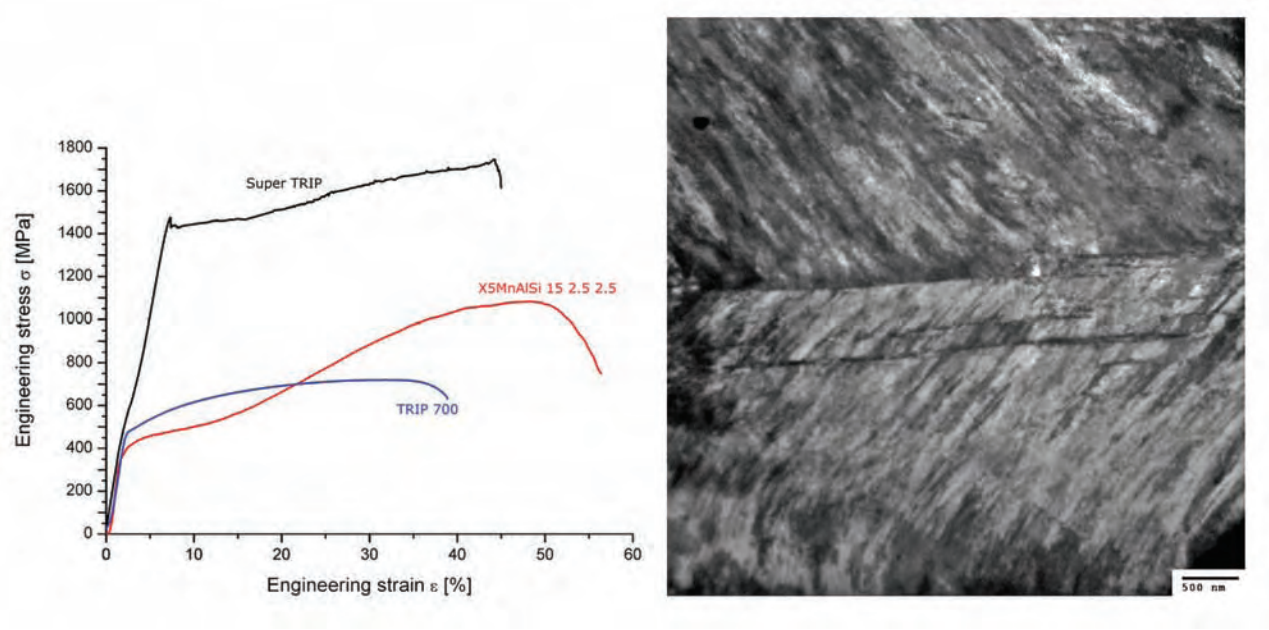

Fig. 2: *Engineering stress strain curves of Super TRIP, X4MnAlSi 15 2.5 2.5 high-manganese m-TRIP, and conventional TRIP 700 steel grades. The TEM bright field image taken from the S-TRIP steel after elongation in tension reveals a high density of the nano-structured α'_{bcc} martensite micro twins.*

The comparison of the stress-strain-curves (Fig. 2) of the X4MnAlSi 15 2.5 2.5 TRIP steel and the conventional residual austenite TRIP 700 steel grade underlines the extraordinary properties such as high plasticity and strength and illustrates the enormous capacity of impact energy absorption. The governing strengthening and deformation mechanism is the severe TRIP effect where a large volume fraction of metastable f.c.c. austenite transformed to α'_{bcc} martensite possessing nano-structured micro twins of high density. The determined average thickness of the twin lamellae is of the order of 30 to 50 nm. The superior strength properties are enhanced by strong solid solution hardening and dispersion strengthening of fine special carbide dispersoids homogeneously distributed throughout the transformed microstructure as shown in the TEM bright field image and the related engineering stress strain diagram of the S-TRIP steel in Fig. 2. Quantitative phase analysis performed by XRD measurements reveal that almost two thirds of the volume fraction of the primary austenite in the as cold rolled sheet sample transformed via strain-induced martensitic transformation to α'_{bcc}.

Newly developed Fe-Mn-Al-C light-weight steels possess lower density up to 15 %, superior strength properties, and high tensile ductility in comparison with conventional deep drawing steels due to their specific alloy compositions, microstructures, deformation and strengthening mechanism. These steels exhibit a triplex microstructure consisting of austenite, ferrite and nano-size κ-carbides of the composition $(Fe,Mn)_3AlC$. The morphology and distribution of these carbides are strongly influenced by the alloying elements; although the thermal treatment may significantly affect their mechanical properties. Pronounced homogeneous shear-band formation causes Shear band Induced Plasticity – SIP effect – and the high strength properties are due to effective solid solution hardening and dislocation interactions in crossing shear bands. The extraordinary ductility and toughness even under impact loading promote high energy absorption at very high strain rates up to 10^3 s^{-1} [4]. Actually, the research is focused on the microstructure evolution in dependence on the alloying elements and the processing parameters. These factors are determining strongly the mechanical properties [5].

The first priority for developing ferritic stainless light-weight steels with medium and higher Al contents is the reduction in specific weight, which is associated with an effective solid solution strengthening caused by the Al additions and sufficient ductility. Up to a limit of about 7 mass% Al the steel shows excellent deep drawing properties. At this Al content a reduction in density of $\Delta\rho$ = 8 % (from 7.87 g/cm³ to 7.25 g/cm³) will be achieved [6]. Another important factor of this class of steel is the material cost reduction by replacing Cr by Al in comparison to conventional ferritic and austenitic stainless qualities where a minimum of 12 or 18 mass% Cr in needed.

The development of particle strengthened ferritic steels for high temperature service in gas turbines is based on experiments and computer simulations of thermodynamics and kinetics of phase transformations. The microstructural evolution and the effect of metastable precipitates on the growth kinetics of stable phases have been studied by means of computer simulations (DICTRA) [7].

The characterisation and optimisation of high-strength light-weight steels were objectives of diverse research projects in cooperation with the steel and automotive industry, supported by the BMBF („Werkstoffentwicklung, Untersuchung und Optimierung der Eigenschaften sowie Bauteilprüfung neuer hochfester supraduktiler TWIP/TRIP-Leichtbaustähle für verstärkende und crashstabile Fahrzeugkomponenten“) and DFG (“Erweiterung der Formgebungsgrenzen“) .

Another subject is the design and evaluation of new high-strength and wear resistant quasi pearlitic steels with sufficient toughness and fatigue properties in the temperature range from -50 to 100 °C. These properties are required for novel steels in modern railway transportation systems and power trains. Quasi eutectoid high-strength and ductile high-carbon steels with aluminium and chromium additions have been developed which fulfil these requirements. The steels possess an ultrafine lamellar pearlite microstructure of sorbite and troostite morphology. In one of the selected highlight papers in Part III of this report (p. 107), the extraordinary high mechanical strength up to the theoretical limit of severely cold drawn wires of this alloy will be presented and discussed in greater detail.

Rapid Solidification Technology

The research group „Rapid Solidification Technology” (J. Gnauk) focuses its activities on the analysis and modelling of solidification processes in general and rapid solidification processes in particular as well as the corresponding process technology and related alloy development.

Both, rapid solidification processes like near net shape casting and welding and industrial scale solidification processes near the local equilibrium do not allow the measurement of all inner occurrences, which are nonetheless often necessary to understand and optimise the appropriate process. Therefore, the calculation of solidification, phase and microstructure formation is an important issue of the activities of the group. The applied models are using the generalised enthalpy method, which allows the computation of heat and mass transfer with multiple coexisting phases. The algorithms are embedded into superordinated FEM and FDM grids to simulate the correct boundary conditions. However, the results quality of the calculation relays strongly on the used fundamental material data.

Hence, the planar flow casting (PFC) facility is used to measure the melt bath geometry and the corresponding temperature distribution to determine kinetic solidification parameters of different metallic melts, using a pyrometric scanner, which was specially constructed for this reason. Other thermophysical

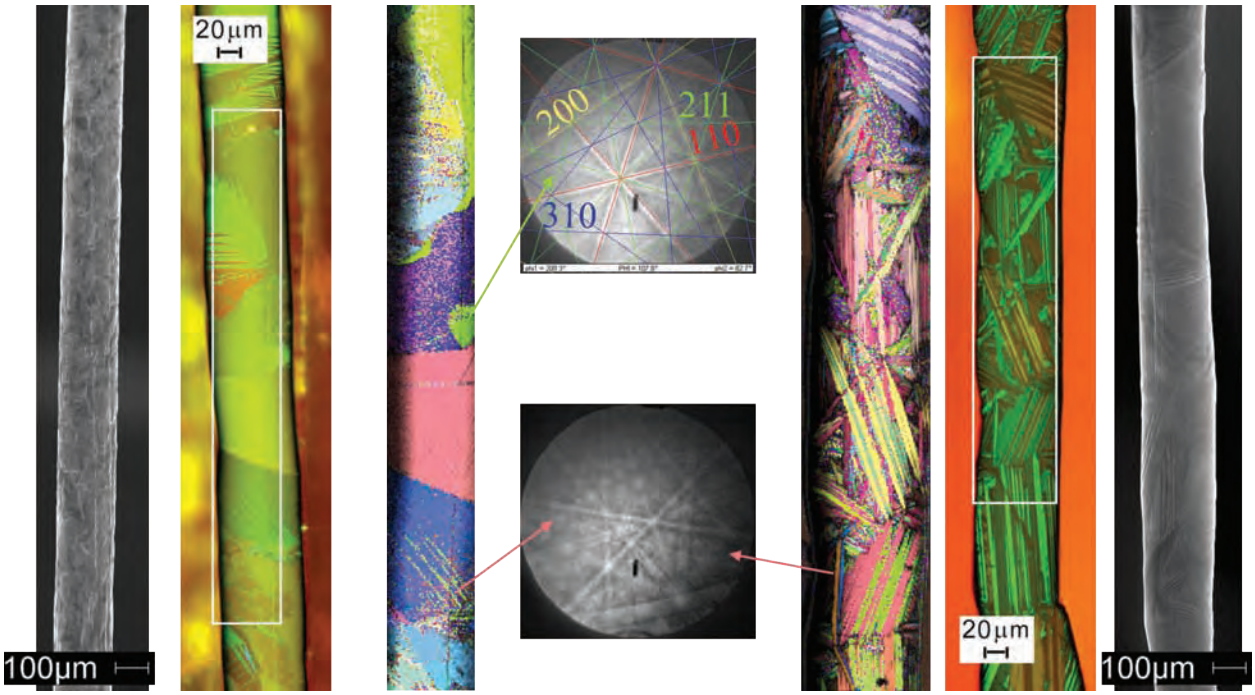

Fig. 3: *SEM and EBSD images of CuAlNi (left) and CuAl (right) shape memory wires. From outside to inside: SEM micrograph showing the surface morphology and microstructures, a colour coded EBSD mapping of the phases and the characteristic Kikuchi patterns exhibit the cubic phase and orthorhombic martensite. Most notable is the homogenous microstructure of the centre and surface section area of the wires.*

properties needed for the calculations are examined in the corresponding facilities of the department.

The phase transformation model is also used to carry out local equilibrium calculations on the solidification of high carbon tool steels during the continuous casting process, which are guided by laboratory scale experiments, simulating CC conditions.

Besides the measurements of the process kinetics, the PFC as well as the other rapid solidification facilities are used to generate rapidly solidified amorphous materials and to freeze in metastable high temperature phases for further characterisation. The “In-Rotation-Liquid-Spinning” (INROLISP) facility was set up to produce rapidly solidified fibres with 50-150 µm in diameter (s. Fig. 3). In addition to the production of high quality softmagnetic microwires, the fabrication of fibres with excellent shape memory properties, which are already present in the as cast state without any former heat treatment are of great and technical interest. Furthermore, the facility can be converted into a shape flow caster (SFC) producing wires of 1-3 mm in diameter directly from the melt [8,9].

Nanoscopic Characterization of New Materials

High performance materials with ordered lattice structures for high-temperature structural applications require a detailed understanding of the influence of the microstructure and the specific defect structures on the atomic scale on their physical and mechanical properties. Therefore complementary to transmission electron microscopy (TEM) atom probe field ion microscopy (APFIM) is used for the chemical analyses of atomic clustering, antiphase boundaries, interfaces, the distribution of solutes and precipitates in the ordered lattices -site preferences- of γ-TiAl, Fe_3Al, FeAl, and NiAl alloys.

Alloys based on the intermetallic B2-ordered NiAl have been investigated regarding the site preferences and precipitation behaviour with ternary additions such as Cr, Fe and Re. Atom probe field ion microscopy (APFIM) was employed to study the site preferences by layer resolved atom probe surveys. The analysis revealed an almost equal distribution of Fe atoms to Ni and Al sites in the sublattices of a NiAl-5 at.% Fe alloy. Cr occupies preferentially Al-sites and showed strong segregation to an ABP of a <111> {123} orientation [10]. The solubility at 1200 °C was determined to be ≤ 1 at.% [11]. Re exhibits a strong preference for the Ni sublattice with a solubility of ≤ 0.18 at.% at 1000 °C [12].

The precipitation behaviour of Cr and Re from the supersaturated NiAl matrix has been analysed. The detailed evolution of the Re precipitates regarding morphology, size, and density in hypoeutectic NiAl-1Re alloy samples annealed at 1000 °C for different times between 10 and 1000 h were investigated by SEM, TEM, and APFIM and in view of the change in the high temperature mechanical properties [12,13]. A 2 at.% Cr containing NiAl base alloy was solution annealed at 1200 °C / 100 h and subsequently age annealed at 550 °C / 500 h. After solution annealing and air cooling the alloy samples exhibited α-Cr particles whereas the annealing at 550 °C resulted in the formation of a Cr-rich so-called X-phase, which has been detected and analysed by APFIM. The atom probe measurement revealed a composition of 16 - 22 at.% Al, less than 0.5 at.% Ni, and Cr in balance. The investigations showed that the solubility of Cr in NiAl is lower than stated in the published phase diagrams, the Cr-solubility is strongly dependent on the Ni/Al ratio, the X-phase is stable at medium temperatures in Al-enriched alloy compositions [14].

A hypoeutectic NiAl-0.6Hf-1.2B alloy particle-strengthened by HfB_2 precipitates has been investigated using APFIM. SEM and TEM investigations could not identify the strong increase of the creep strength observed in this alloys after an annealing at 1300 °C/100 h. However, FIM analysis revealed a relatively high density of boron-atom clusters as well as needle shaped particles with a maximum size of 4 x 15 nm, as shown in Fig. 4 (next page). Atom probe analysis revealed that the smallest clusters consist of about 5 to 20 boron atoms and larger ones contained up to 200 atoms. The boron enrichments can be described as boron decorations at lattice defects like vacancies or planar faults comparable to Cottrell cloud formation [15].

Comprehensive investigations including single atomic layer resolved APFIM investigations, ALCHEMI (Atom Location Channelling-Enhanced Microanalysis) and X-ray diffraction have been performed to determine the site preference and the lattice distortions due to the dissolved transition metals V, Nb, Cr, Mo, and Cu in γ-TiAl with the ordered f.c.t. $L1_0$-type of lattice structure.

Chromium or copper atoms exhibit a strong site preference for the Al sublattice depending upon the aluminium concentration. In contrast vanadium or niobium atoms are located in the Ti sublattice where the site preference of the alloying additions is almost 100 % [16]. Molybdenum atoms are equally distributed over both sublattice sites.

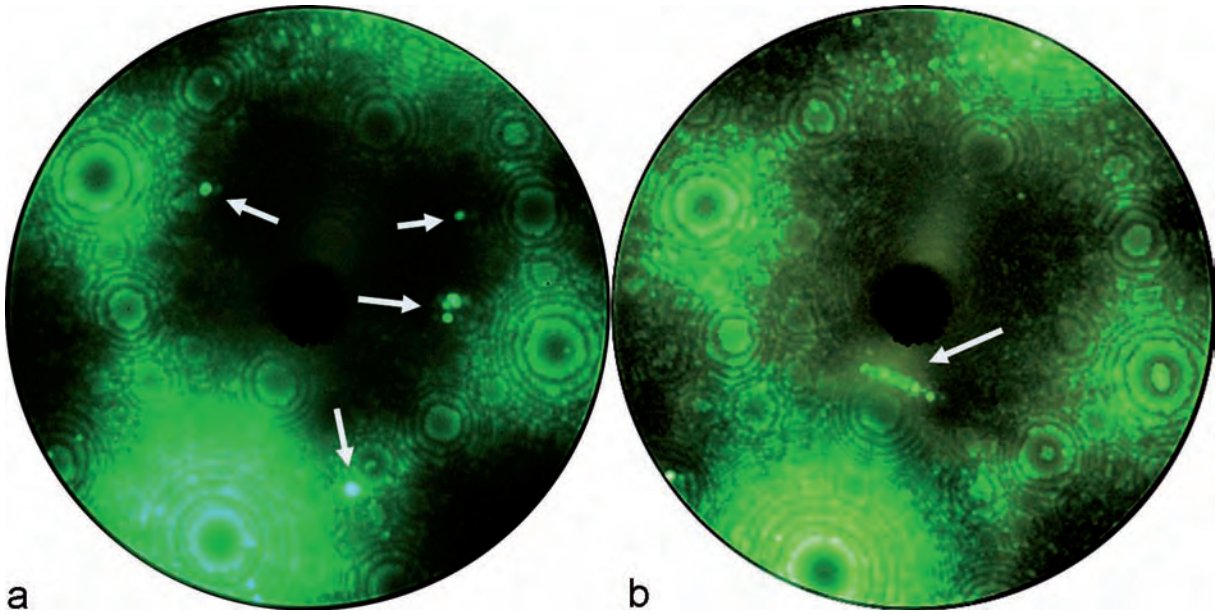

Fig. 4: *Field-ion micrographs revealing two different types of boron enrichments (brightly imaged). Nanoscopic boron clusters of high atomic density are presented in (a). A needle-shaped boron enrichment was detected near the {013} pole (b).*

Mo atoms slightly decrease the lattice parameters a and c to the same amounts, so that the c/a ratio remains unchanged, whereas Cu atoms lower the a parameter more strongly than the c parameter. This results in a relative increase of the c/a ratio.

The alloying elements also influence the atomic densities of the γ-TiAl unit cells. Additions of Cr, V, Mo and Cu decrease the atomic densities of γ-TiAl where Cr atoms cause the strongest effect on the atomic density of the f.c.t. unit cell [17].

Ordered Alloys for High-Temperature Application

Ordered alloys based on aluminides, silicides and refractory Laves phases are potential candidates for engine components exposed to high-temperature and corrosive environments in energy conversion systems, such as internal combustion engines, jet engines, steam turbines, stationary gas turbines and heat exchangers in power plants with improved thermal efficiency.

Iron-, nickel- and titanium aluminides with cubic B2 or $D0_3$ and tetragonal $L1_0$ superlattice structures as well as the high melting point silicides and Laves phases with complex hexagonal $D8_8$, orthorhombic C54 or cubic C15, and hexagonal C32 types of lattice structures enable a large variation in alloy design to achieve superior physical and mechanical properties, such as high elastic stiffness, improved warm and creep strength and excellent hot gas corrosion and oxidation resistance. A great challenge is the improvement of fracture toughness at room and lower application temperatures.

Gamma titanium aluminides are the most promising high-temperature light-weight material alternative to heat-resistant steels and superalloys because of the low specific weight (3,8 gcm^{-3}), high elastic stiffness - Young's modulus of about 176 GPa -, and considerable tensile strength of R_m > 800 MPa. In addition γ-TiAl based alloys show excellent oxidation resistance up to 800 °C. Due to their properties profile γ-TiAl based alloys have intensively been investigated worldwide and are already in technical service for high performance components such as compressors and valves in combustion engines and are technically evaluated for structural components in instationary and stationary gas turbines.

Comprehensive structural characterisation of two-phase γ-TiAl/α_2-Ti_3Al exhibits enhanced room temperature ductility which is due to dislocation glide and mechanical twinning, because of the relatively low stacking fault energy of gamma aluminide [17-20]. The site preferences were determined by high resolution APFIM and ALCHEMI analysis in collaboration with Vanderbilt University and Oak Ridge National Laboratory [20]. The fine-grained equiaxed microstructure of the two-phase alloys reveals structural superplasticity. At temperatures of 950 to 1000 °C strain-rate-sensitivity exponents of m = 0.5 were recorded. In superplastic strain to failure tests about ε_{pl} = 1000 % uniform elongations at strain rates of 10^{-2} s^{-1} were achieved [21,22].

One important class of materials are nickel aluminides alloyed with the refractory b.c.c. and h.c.p. metals Cr, Mo, and Re. Quasi binary hypoeutectic and

directionally solidified eutectic systems have been investigated with respect to mechanical properties, such as elasticity, solid solution hardening, fibre reinforcement, creep strength and fracture toughness in view of atomic defects and microstructural features [23-25]. Among the investigated alloys the unidirectionally solidified fibre reinforced NiAl-(Mo,Re) eutectic composites possess optimum high temperature strength and creep resistance up to 1300 °C where as the chromium containing material exhibits a good combination of strength and ductility up to 1200 °C [24,26]. To tap the full potential of maximum application temperatures NiAl was particle strengthened by the high melting point TiB_2, ZrB_2, or HfB_2 diborides. Constitutional investigations reveal each single system to be quasi-binary eutectic (Fig. 5) with eutectic temperatures of T > 1630 °C [27]. In comparison to single phase NiAl the particle strengthened NiAl-based alloys are characterized by higher plastic elongation in compression testing at room temperature as well as increased high temperature strength and creep resistance [28].

A rapidly solidified and thermomechanically processed fine-grained eutectic NiAl-Cr alloy of the composition $Ni_{33}Al_{33}Cr_{34}$ exhibits structural superplasticity in the temperature regime from 900 °C to 1000 °C at strain rates ranging from 10^{-5} to 10^{-3} s^{-1}. The material consists of a B2-ordered intermetallic NiAl(Cr) solid solution matrix containing a fine dispersion of b.c.c. chromium. A high strain-rate-sensitivity exponent of m = 0.55 was achieved in strain-rate-change tests at strain rates of about 10^{-4} s^{-1}. Maximum uniform elongations up to 350 % -engineering strain- were recorded in superplastic strain-to-failure tests. Activation energy analysis of superplastic flow was performed in order to establish the diffusion-controlled dislocation accommodation process of grain boundary sliding. An activation energy of $Q_c = 288 \pm 15$ kJ/mole was determined. This value is comparable with the activation energy of 290 kJ/mole for lattice diffusion of nickel and for ^{63}Ni tracer self-diffusion in B2-ordered NiAl. The principal deformation mechanism of superplastic flow in this material is grain-boundary sliding accommodated by dislocation climb controlled by lattice diffusion which is typical for class II solid-solution alloys. Failure in superplastically strained tensile samples of the fine-grained eutectic alloy occurred by the formation of cavities along NiAl || Cr interfaces [29].

Advanced high melting point silicides with low density have been evaluated because of their potential applications at 1300 °C and above. The refractory titanium silicides Ti_5Si_3 and $TiSi_2$ with complex hexagonal $D8_8$ and orthorhombic C54 lattice structures exhibit superior physical and mechanical poperties, such as high lattice energies and melting temperatures; high hardness, elastic stiffness and flow stresses; low densities and excellent creep and oxidation resistance. The complex lattice structures and the governing covalent bonding of these compounds cause a lack in ductility due to sessile superdislocations. The ductility and fracture toughness of the silicides have been considerably improved by adding aluminium to the refractory compounds and by producing nanosized grain structures. However, optimum creep strength at 1300 °C occurs in coarse grained silicides [21].

Structures and stability of cubic and hexagonal Laves phase polytypes have been investigated in a number of fundamental studies on various binary and ternary phase diagrams [30-34]. In two review papers, the structure type variations of Laves phases observed in many systems and the factors controlling the structure and stability of Laves phases have been critically discussed [35,36]. In the beginning of 2006, the inter-institutional research initiative “The Nature of Laves Phases” has started. This networking project is a co-operation between the MPI for Chemical

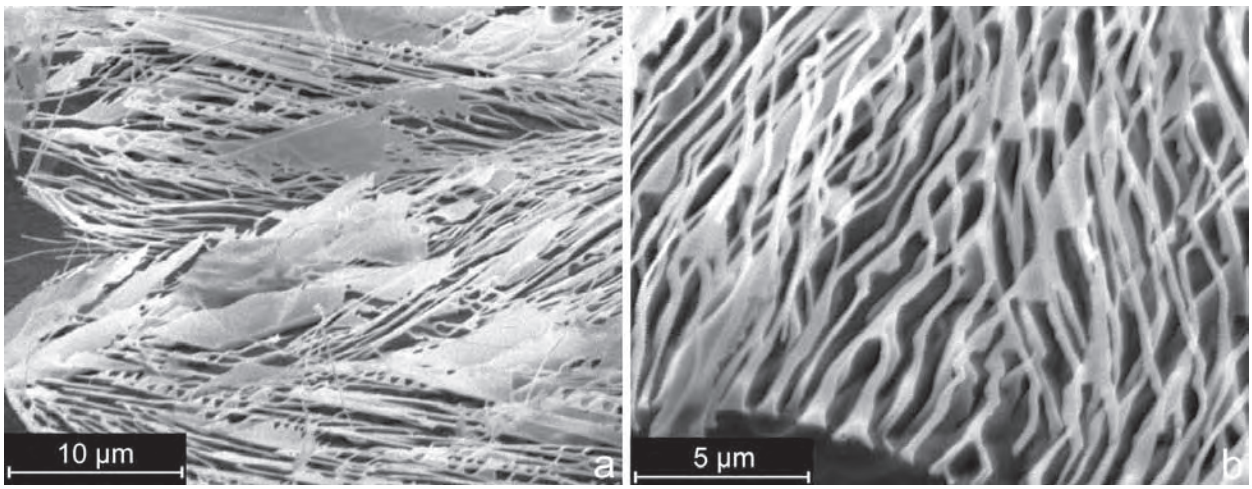

Fig. 5: *SEM images of the microstructure of the NiAl-0.75Hf1.5B eutectic in the as-cast condition. By partial etching of the NiAl matrix a detailed view of the fibrous microstructure and its eutectic growth faults are revealed: lamellae (a) within the fibrous microstructure and branching faults (b).*

Physics of Solids in Dresden, the MPI for Solid State Research and MPI for Metal Research both in Stuttgart, and the MPIE. The aims of this research initiative are described in detail on page 17 in Part I of this report.

Laves phases play an important role in strengthening novel intermetallic-based materials at high temperatures. Therefore their strengthening effect and deformation behaviour has been studied in a number of Fe-Si- and Fe-Al-based systems [37-40]. The principal strengthening mechanisms available for Fe-Al-based alloys and their individual contributions for strengthening at elevated and high temperatures have been reviewed [41,42] and based on this critical analysis aimed alloy developments have been carried out which led to Fe-Al-based materials with significantly increased creep resistances [40,43-46]. Like other high-strength materials these Fe-Al-based materials show only a limited ductility at room temperature and ambient temperatures. In order to identify the factors which cause this embrittlement, a systematic study of the brittle-to ductile transition temperatures in dependence of the aluminium content has been carried out [45]. As the ductility is also affected by vacancies and impurities such as carbon, they have been studied by investigating the anelastic relaxation in Fe-Al-(Ti, Nb) alloys by mechanical spectroscopy, positron annihilation spectroscopy and by radio tracer diffusion [47]. The early stages of the formation of protective oxide layers has been studied by combined X-ray photoelectron spectroscopy (XPS), grazing incidence XRD with synchrotron radiation and transmission electron microscopy (TEM) [48]. All these activities are part of the inter-departmental research activity on “Innovative Fe-Al-based materials” which is described in greater detail on page 113 of this report.

Iron aluminium alloys are regarded as promising for high temperature application under carburisation conditions. The reason for this is the observation of a thin alumina layer which forms at very low oxygen potentials in gaseous atmosphere and could be used as protective against carburisation and following metal dusting. The investigation of carburisation and metal dusting in a flowing H_2-CO-H_2O gas mixture at 600°C on Fe-xAl (x = 15, 26, 40 at. %) were carried out at carbon activities of a_C = 275 and a_C = 405. The thermogravimetrical analysis (TGA) shows increasing carburisation kinetics with increasing carbon activity of the gas mixture for the alloys with the same Al content. The higher the Al content of the alloys the slower the carburisation reaction is and metal dusting sets on at later times. XPS and SEM investigations of the surface show that the retardation of metal dusting depends mostly on the integrity of the alumina scale. At a_C = 405 the precipitation of κ-phase Fe_3AlC with perovskite structure was detected on an Fe-15Al sample [49].

Intermetallic phases also offer the possibility to develop new light-weight materials as many phases of low density exist which in addition show high melting points, good mechanical strength and partly an excellent corrosion resistance. In order to exploit the potential of these phases, the phase diagrams for the Al-Ti and Al-Mo system have been assessed in a first step [50,51]. Based on the results obtained from the assessment of the Al-Ti system a large scale joint project between the University of Magdeburg, ACCESS e.V. (Aachen), Caesar (Bonn), and MPIE funded by the Deutsche Forschungsgemeinschaft (DFG) has been started in 2006. Within this project phase transformations which yield specific microstructures are analysed and the effects of these microstructures on mechanical properties are subject of ongoing research activity.

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Research Projects in Progress

Innovative Steel Research

Frommeyer, Brokmeier, Rablbauer: Structural investigations on Super TRIP steels

Frommeyer, Brokmeier: Development and evaluation of quasi eutectoid high carbon-aluminium steels

Frommeyer, Gnauk: Industrial up-scaling of the Mn-Al-C steel metallurgy

Frommeyer, Gnauk: Superplastic alloys used as intermediate bonding layer in the cladding by the rollbending process.

Frommeyer, Rablbauer: Development and Characterisation of ultrahigh strength pearlitic steel wires

Frommeyer: Investigations on the mechanism of martensitic transformations in iron carbon steels

Gnauk, Frommeyer: Development of resistible soldering alloys for high strength steels

Gnauk, Frommeyer: Modelling of centre segregation and carbide formation during the continuous casting of ledeburitic tool steels

Gnauk, Frommeyer: Reduction of core segregation in continuously cast ledeburitic tool steels

Maier, Rablbauer, Frommeyer: Investigations on plastic deformation behaviour in TRIP steels

Rablbauer, Engberding: Microstructure, phase stability, and mechanical properties of phosphorus microalloyed TRIP and TWIP steels

Rablbauer, Frommeyer: Development and characterisation of ferritic stainless Al-Cr steels of deep drawing quality

Rablbauer, N.N., Frommeyer: Alloy composition and thermomechanical processing optimization of Mn-Al-Cr steels

Rablbauer, N.N., Frommeyer: Fundamental investigations on the plastic deformation mechanisms of carbide particle strengthened Mn-Al-C steels

Stein, Frommeyer: Fe-Si alloys with 3.5 to 6.5 wt.% Si processed under microgravity

Rapid Solidification Technology

Gnauk, Frommeyer: Development of alloying systems for flux free soldering of aluminium alloys

Gnauk, Wenke: Macroscopic modelling of phase formation and microstructure evolution in aluminium-steel joining interfaces

Gnauk, Wenke: Modelling of phase and microstructure formation under non-equilibrium conditions of aluminium-titanium laser welded seams

Gnauk, Zeller, Frommeyer: Continuous casting of soft magnetic fibres for new magnetic field sensors

Wenke, Gnauk: Investigations on melt pool undercooling of aluminium alloys during the meltspinning process

Zeller, Gnauk: Investigations on continuously cast fibres and wires of Cu-based shape memory alloys

Development and Characterisation of New Materials

Engberding, Palm, Stein: Transformation of h-Al_2Ti and Al_5Ti_3 and the formation of lamellar TiAl + r-Al_2Ti microstructures

Frommeyer, Rablbauer: Structural superplasticity in fine-grained NiAl-Mo alloys

Frommeyer, Wittig (*Vanderbilt University, TN, USA*): Development of ductile chromium based alloys for high-temperature application and microstructural characterization

Gnauk, Frommeyer: New alloys for laser diode heat sinks

Krein, Palm: Development of Fe-Al alloys on the basis of Fe_3Al for application at elevated and high temperatures

Milenkovic, Palm, Frommeyer: Directional solidification of Fe-Al-Nb alloys

Palm, Krein, Brunetti, Hazotte*, Grosdidier* (Univ. Metz)*: Brittle-to-ductile transition temperatures (BDTT) of ternary Fe-Al-X alloys

Palm, Morris (CENIM, Madrid), Lacaze (CIRIMAT, Toulouse): Innovative Fe-Al alloys for demanding applications

Palm, Schuster, Weitzer* (*Univ. Wien)*: The Fe-Si-Ti system

Palm, Stein, Engberding, Heilmaier, Saage*, Sturm* (*Univ. Magdeburg), Drevermann**, Paninski**, Schmitz** (**Access eV, Aachen), Kelm***, Quandt*** (***caesar, Bonn)*: Al-rich AlTi alloys

Prymak, Stein, Palm: Phase equilibria in the Nb-Al-X (X = Cr, Fe, Co) systems

Rablbauer: Development of Fe_3Al-based constructional materials for power train application

Rablbauer, Deges, Frommeyer: Fundamental research on physical and mechanical properties of Fe_3Al-Cr solid solution single crystals

Spiegel, Stein, Liapina: Initial stages and kinetics of oxidation of binary and ternary iron-aluminides

Stein, Palm, Sauthoff, Raabe, Frommeyer, Kreiner, Grin* (*MPI-CPfS, Dresden), Leineweber**, Mittemeijer** (**MPI-MF, Stuttgart), Fischer***, Jansen*** (***MPI-FKF, Stuttgart)*: MPG Research Initiative: The nature of Laves phases

*Stein, Palm, Vogel** (*LANL, Los Alamos): Investigation of crystal structures at high temperatures by neutron diffraction

Stein, Palm: DTA studies of phase transitions in the Fe-Al system

Stein, Prymak, Palm, Kreiner, Siggelkow* (*MPI-CPfS, Dresden)*: Phase stability and mechanical behaviour of Co_7Nb_2

Department of Microstructure Physics and Metal Forming

D. Raabe

Scientific Mission

The Department of Microstructure Physics and Metal Forming conducts fundamental and applied research on the relationship between processing, microstructure, and properties of structural materials with special emphasis on steels. Advanced characterization and basic theoretical understanding of microstructure evolution under complex thermomechanical history and boundary conditions and its relevance for the mechanical behaviour play key roles in our research strategy. In most projects we pursue a close integration of theory and experiment (Fig. 1). Six main competence groups form the cornerstones of the department, namely,

- Theory and Simulation (F. Roters)
- Diffraction and Microscopy (S. Zaefferer)
- Thermomechanical Processing (D. Ponge)
- Metal Forming (until 2007) (W. Rasp)
- Leibniz group on Biological Materials (since 2005) (D. Raabe)
- Max-Planck-Fraunhofer Initiative on Computational Mechanics of Polycrystals (since 2006) (P. Eisenlohr)

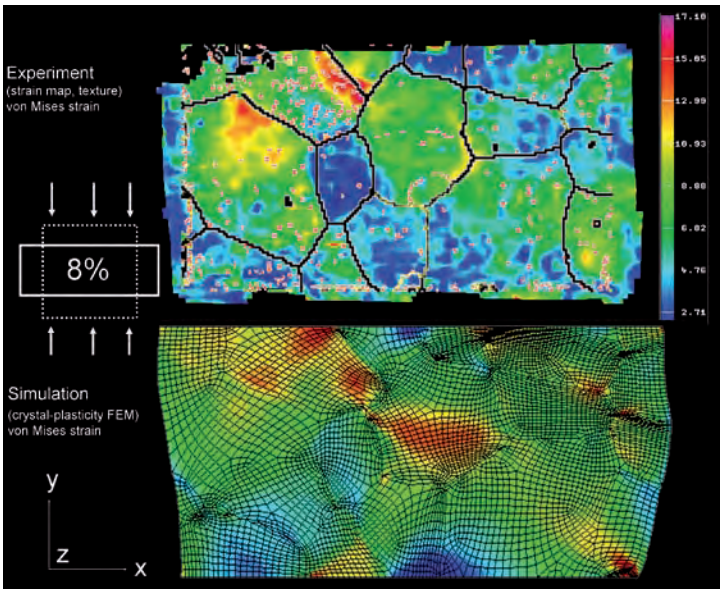

Fig. 1: *Most projects in the department are characterized by a very close integration of experiment and continuum-based crystal-plasticity simulation. The figure shows the heterogeneous strain pattern observed experimentally in a plane-strain loaded polycrystal (pure Al, columnar grains) together with a simulation which was conducted by using a viscoplastic crystal plasticity finite element method. The colour code indicates the von Mises equivalent strain (experiment, simulation). The black lines in the upper figure (experiment) indicate the grain boundaries as measured by electron back scatter diffraction.*

As a rule these competence groups work closely together. This means that most projects in the department, which will be discussed in more detail below, are usually not designed and conducted by one group alone but by two or three teams together. The table presents the most important research fields in the department during the past six years.

Main research highlights in the years 2001 – 2006
Crystal mechanics (theory and experiment) for very small scales (sub-grain scale, e.g. nano-indentation) and for very large scales (10^9 grains, e.g. automotive sheet forming)
Connection between internal variable-based constitutive models and the simulation of deformation-induced damage nucleation
Multiphase 3D EBSD nano- and microtexture analysis via the integration of joint focussed ion beam and electron back scatter diffraction microscopy
Microstructure, processing, and properties of steels with a ultrahigh density of interfaces
Structure, crystallographic texture, and properties of biological nanocomposites

In addition to these scientific competence groups the department has established five service groups, namely, “Scientific Computing and Computational Services”, “Metallography”, “Materials Testing Laboratory”, “Micromechanics Laboratory” and “Materials Processing”. The basic idea behind this structure of the department is to build a highly interdisciplinary research initiative which aims at merging physics-oriented microstructure research and materials processing on the one hand and theory and experiment on the other hand.

Theory and Simulation (F. Roters)

Mission. The main research focus of the group Theory and Simulation is the development of physics-based constitutive models for the micromechanical behaviour of materials. The Finite Element Method (FEM) serves in most projects as the standard tool for solving the coupled sets of partial differential equations which map the plastomechanical behaviour of materials under external loads. The development of constitutive models which replace the common empirical hardening laws in this field by internal variable formulations which are built on rate equations for tracking the evolution of mobile, sessile, and geometrically necessary dislocation populations and the evolution of and mechanics at internal interfaces has in the six past years been the main task of the group (Fig. 2).

Recent highlights. The work of the group Theory and Simulation in the years 2001 – 2006 has mainly focused on two topics, namely, on the application of crystal plasticity theory to small scales and to large scales. The first group of projects (crystal plasticity at small scales) is concerned with the development of advanced physics-based constitutive laws which root in dislocation dynamics on the one hand and on grain boundary mechanics on the other as two main internal variable sets required for the improvement of the foundations of the crystal plasticity finite element method. These improved constitutive laws are required to tackle small scale crystal plasticity issues such as gradient and contact effects as well as grain boundary mechanics [1-11].

The second area is the further development of the crystal plasticity finite elements method for large scale applications in the form of different variants of texture-function-based crystal plasticity finite element methods [12-15]. These approaches basically form a combination of either the texture component method or Fourier-based pole figure inversion approximations with the crystal plasticity finite element method. The aim of these methods is to solve the key problem of incorporating anisotropic material behaviour into industry scale finite element simulations, namely, to formulate an efficient way for representing crystallographic texture and its evolution in forming simulations. The texture function finite methods are very well suited for this purpose.

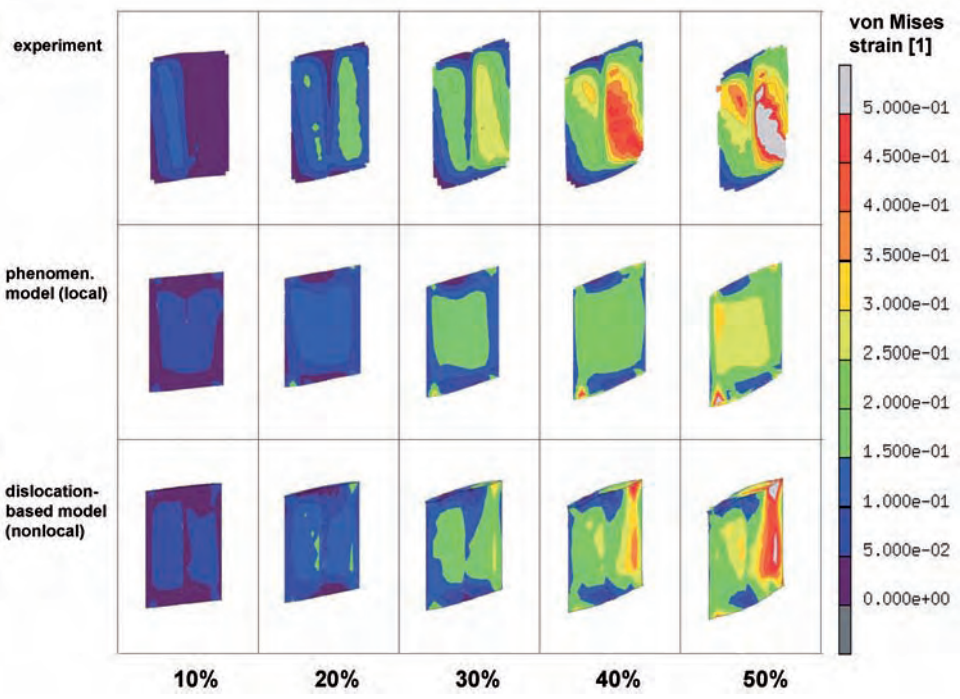

Fig. 2: *Upper row: strain mapping experiment (Von Mises strain measure) for a sheared bicrystal (no friction effects) with a [112] low angle tilt grain boundary (pure Al). Middle row: crystal plasticity finite element simulation of the same experiment using a conventional viscoplastic hardening law. The simulation was not sufficiently successful since it does not capture the effect of the interface on the overall mechanics of the sample as indicated by the absence of load sharing among the abutting crystals. Bottom row: crystal plasticity finite element simulation of the same experiment using a novel dislocation-based hardening law. The simulation was successful since it captures the effect of the interface on the overall mechanics of the sample.*

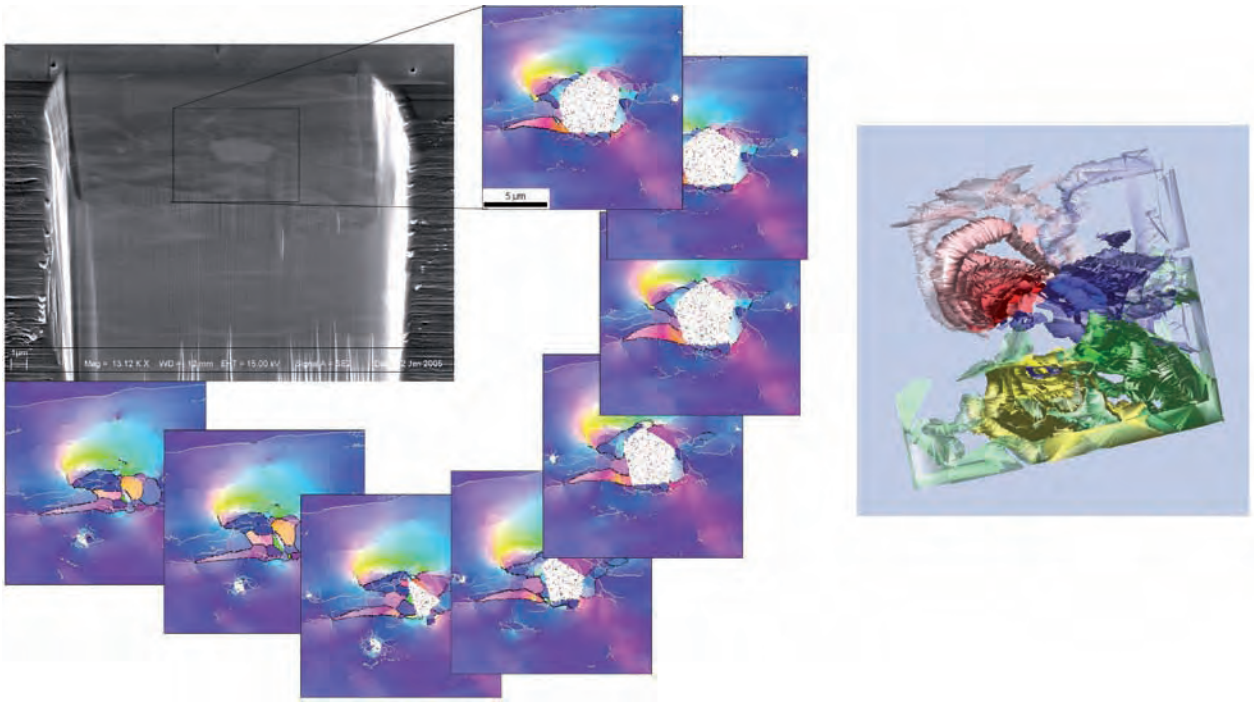

Fig. 3: *Example of the serial sectioning method employed in the 3D EBSD system around a hard Laves phase embedded in a plastically strained Fe_3Al intermetallic matrix. The focussed ion beam (FIB) microscope is used to conduct series of sections (300 nm spacing in this case) and the EBSD system tracks in each slice the crystallographic orientation (colour code). The image on the right hand side shows the topological reconstruction of the crystallographic orientation gradients that surround the hard inclusion. The orientation gradients are presented in terms of four different colours according to the local reference orientation at the actual interface. Each misorientation layer which is indicated by the weakening colour gradient represents a change in orientation of 5° between the orientation layers [25,26].*

Instead of hundreds of individual orientations, as they are frequently used in other texture discretisation procedures, it uses either very few Gaussian texture components or Fourier coefficients for decomposing the experimentally obtained starting texture in a crystal plasticity finite element mesh via a statistically weighted mapping procedure.

Microscopy and Diffraction (S. Zaefferer)

Mission. The main mission of the Microscopy and Diffraction group consists in the experimental investigation of the microstructure and crystallographic texture in complex multiphase materials [16-24]. The focus lies on the investigation of local metallurgical processes such as athermal transformation and interface crystallography or recrystallization nucleation. Therefore, the experimental methods mainly comprise transmission and high resolution scanning electron microscopy (TEM and SEM) together with the corresponding diffraction techniques (transmission Kikuchi and spot diffraction in the TEM and 2D as well as 3D backscatter electron diffraction (EBSD) in the SEM or in the FIB-SEM, respectively, Fig. 3). Additionally, X-ray diffraction is used to measure textures, single grain orientations and residual stresses on a macroscopic and microscopic scale.

The group is equipped with a variety of instruments for microstructure and microtexture characterization. The most recent and essential acquisition is a high-resolution Zeiss Crossbeam XB1560 FIB for 3D EBSD investigations. This machine is a combination of a high resolution SEM and a focussed ion beam (FIB) microscope equipped with a TSL EBSD system and EDX. For 2D EBSD investigations, a high-resolution, high-beam SEM (JEOL JSM 6500 F) with a TSL EBSD system as well as a standard tungsten filament SEM (JEOL JSM 840A) with an HKL Technology EBSD system is available. All types of SEM instruments allow one to mount micro-tension machines of different dimensions for in-situ deformation tests. 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 (S. Zaefferer) for on-line crystallographic analysis. Furthermore, an X-ray goniometer equipped with capillary beam guide for high X-ray intensity and an area detector is available. Alternatively, this instrument can be used with a monochromator set-up for high-precision residual stress measurements.

Recent highlights. The most important current project in the group is the development of a novel multiphase 3D EBSD nano- and microtexture analysis method via the integration of joint focussed ion beam

and electron back scatter diffraction microscopy. This is realized by using a Zeiss Crossbeam XB1560 FIB which is a combination of a high resolution SEM and a focussed ion beam (FIB) microscope. While the SEM part is used to observe and analyse the sample, the FIB part serves to cut and structure the sample surface. One particular application is the 3D orientation approach which works by a serial sectioning technique. By this method, orientation resolutions of about 503 nm^3 are achieved and material volumes of about 50 x 30 x 30 μm^3 can be probed. Besides standard electron detectors the instrument is also equipped with a transmitted electron detector for the acquisition of scanning transmission electron images from thin foils. These foils are made by cutting with FIB at well defined positions.

Thermomechanical Treatment (D. Ponge)

Mission. The aim of the group for Thermomechanical Processing is the basic investigation of the relationship between the processing, the microstructure, and the mechanical properties of steels [27-35]. The characterization and the basic understanding of the mechanisms which guide the observed microstructures under complex thermomechanical history and boundary conditions and their relevance for the observed micro- and macromechanical behaviour is the key area of all projects in this group.

Experiments are conducted by using a variety of casting and large scale forming devices, such as the 2.5MN hot compression machine. This servohydraulic press is capable of conducting large-scale thermomechanical processes by performing multi-step hot compression tests as a realistic approximation of industry-scale hot forming operations. Characterization is conducted by applying the full spectrum of experimental techniques available in the institute including deformation dilatometry, electron microscopy, and mechanical testing.

Recent highlights. The key projects in the past six years in this group were dealing with ultra fine grained steels [31-35]. Microstructures comprising fine ferrite grains and dispersed cementite particles for plain C-Mn steels (with different contents of C and Mn) have been achieved by controlled cooling and heavy warm compression on a 2.5MN hot compression set-up. The final re-coiling has also been investigated as an important step for large scale production. The grain boundary character distribution created in such steels was investigated by using electron backscattering diffraction (EBSD): The fraction of high angle grain boundaries (disorientation angle $\omega \geq 15°$) was found to be approximately 60% in the ferrite. Considering only high angle grain boundaries the average ferrite grain size amounted to only 900 nm. If all grain boundaries ($2° \leq \omega \leq 63°$) are considered, the mean ferrite (sub)grain size was only 600 nm. The hardness increases with decreasing grain size. Dispersed fine cementite particles were found to be very efficient in preventing ferrite growth (Fig. 4). A second set of projects investigated novel process routes which entailed ultra fine microstructures which were formed by thin slab casting combined with direct rolling strategies in the austenitic regime.

Metal Forming (W. Rasp)

Mission. The main objective of this group is the theoretical analysis and accompanying experiments in the field of forming processes placing emphasis on hot and cold rolling [36,37]. Projects are based on

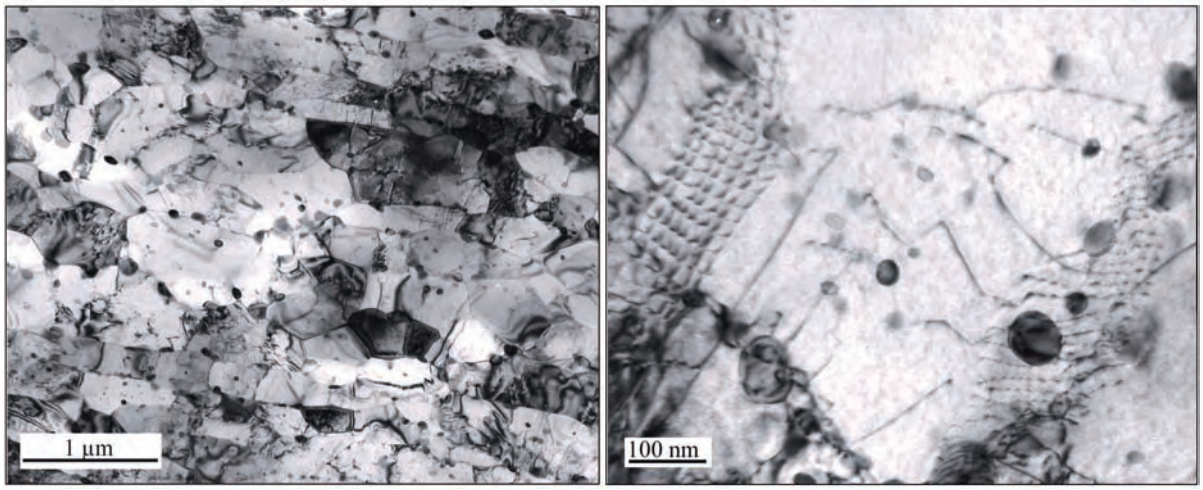

Fig. 4: *Ultra fine grain structure obtained for a conventional 0.2wt.% C-Mn steel. The microstructure was formed by imposing four subsequent deformation steps each at a true (logarithmic) strain of 0.4 at a temperature of 823 K, followed by a 2 h holding time at 823 K to mimic hot coiling. The average grain size obtained by this method was below 1 µm which is extremely fine for a commercial C-Mn steel grade. Typically steels of this grade have a grain size which is 10 times larger [31-35].*

plastomechanical, elastomechanical, and tribological fundamentals in order to study forming processes under the complex boundary conditions typically imposed by the workpiece-interface-tool system. After the retirement of the current group leader, Dr. Rasp, a new group with a modified mission will be opened in 2007.

Recent highlights. The key project in the Metal Forming group in the past six years was a study on the improvement of formability of brittle materials by a superimposed hydrostatic pressure. The experiments were performed by a simultaneous deformation of a brittle core material and a ductile shell surrounding the core. The deformation of the shell is a forward-extrusion process. By varying the shell material and the deformation degree the hydrostatic pressure acting against the core material can be increased up to the limits of the tool and press. With this method the formability of brittle core materials can be studied.

Leibniz Group on Biological Nano-Composites (D. Raabe)

Mission. The main objective of this new group is the basic study of the internal structure and the corresponding micromechanical behaviour of biological materials [38-42]. The current emphasis is on chitin-based materials such as encountered in the exoskeleton of arthropods and collagen-based materials such as bone. Particular attention during the past 2 years since this initiative exists has been placed on the investigation of the structure and the mechanical properties of crustaceans, mainly of *homarus americanus* (lobster). This material is an excellent example of a bio-nano-composite with variable properties and substantial structural and mechanical anisotropy which manifests itself both, at the microscopic and at the macroscopic scale. As in most mineralized natural polymer tissues, the mineral components of the crustacean shell are associated with complex organic matrices which include proteins, glycoproteins, polysaccharides and lipids. The most important polysaccharide in the cuticle of lobster and crab (as in insects) is α-chitin, a cellulose-like crystalline biological polymer.

Recent highlights. During its first 2 years the newly established group, which is funded by the German Research Foundation DFG through the Gottfried Wilhelm Leibniz award, has been concerned with experiments for a better understanding of the mesostructure and microstructure of the exoskeleton of homarus americanus and their relevance for the mechanical properties observed. The investigations have concentrated on the structure and the mechanics of the lobster claw and carapace. For the structure and microstructure characterization experiments we used light optical transmission microscopy, laboratory-scale X-ray diffraction in conjunction with an area detector, synchrotron-based phase and texture analysis at DESY and DELTA, high resolution scanning electron microscopy, and transmission electron microscopy. In order to identify all different components in the material, some of them were gradually removed by tailored chemical etching. The microstructure of the lobster cuticle was then observed after the subsequent removal of certain parts of the organic matrix, mainly of the proteins, and after the removal of the mineral phase, respectively. The observed structures are used for the interpretation of the mechanisms that govern the mechanical properties of the material (Fig. 5). During the last months a project has been initiated to design a micromechanical model for understanding the origin of the observed structure-property relationships of such nanocomposites. The approach is built on a

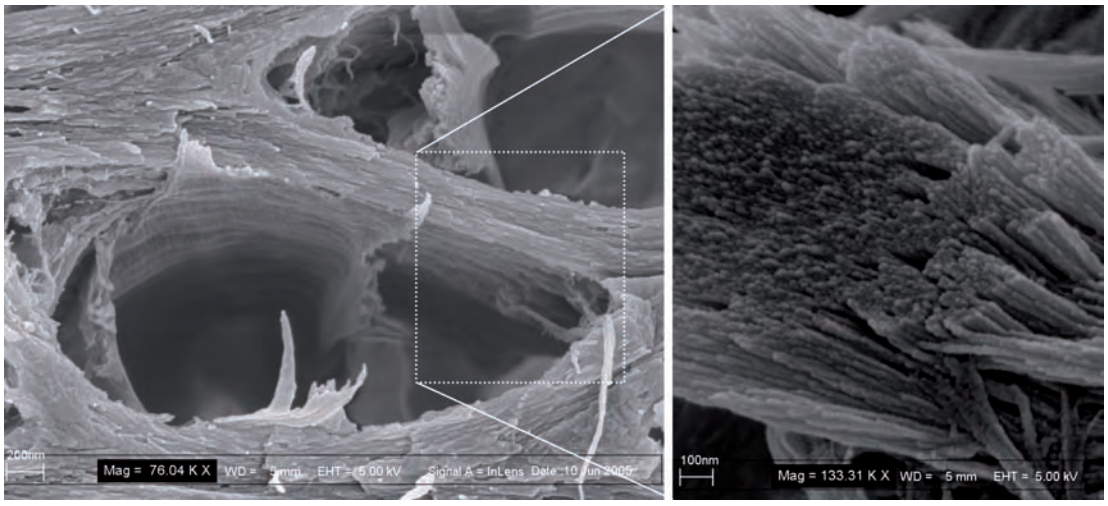

Fig. 5: *SEM-micrograph of the inner structure of the mineralized chitin-protein fibre layer in homarus americanus. The image on the left hand side reveals that the inner structure of the material resembles a honeycomb arrangement. The fibres consist of many tiny filaments (see image on the right hand side) [38-42].*

hierarchical version of an Eshelby-type multiphase self-consistent homogenization method.

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

Mission. The new research initiative on Computational Mechanics of Polycrystals which was established in October 2005 as the first ever joint research group between the Max-Planck-Society (Department of Microstructure Physics and Metal Forming at the Max-Planck-Institut für Eisenforschung, Düsseldorf) and the Fraunhofer-Society (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg) pursues the idea to develop and enhance novel theoretical approaches for the field of mechanics and damage nucleation of crystalline matter with the aim to promote its use for industrial applications such as encountered in the fields of aerospace, automotive, and medical engineering.

Recent highlights. The new group on Computational Mechanics of Polycrystals deals with all relevant challenges associated with crystal plasticity finite element simulations of the microstructure evolution and mechanical response of complex metallic multiphase materials with respect to engineering applications. In terms of metal physics the group places its current focus on the micromechanical fundamentals associated with multiphase mechanics, deformation induced phase transformations, deformation twinning, and strain-induced damage nucleation. In terms of the computational and engineering challenges associated with the field of crystal plasticity the group currently aims at developing, optimizing, and accelerating appropriate numerical and homogenization schemes to lead the field of computational mechanics of polycrystals to rapid industrial maturity. Details of this initiative are given in a separate chapter of the scientific report.

Spirit, Teamwork, Outreach, Achievements

All projects in the department are pursued in an interdisciplinary and team-oriented spirit. Scientists in our department come from such different fields as theoretical and experimental physics, materials science and engineering, metallurgy, biology, chemistry, theoretical mechanics, mechanical engineering, polymer physics, and polymer mechanics, i.e. communication is paramount to the scientific success of the group. Projects are pursued in an atmosphere of mutual learning, inspiration, and interdisciplinary co-operation including in particular an intense exchange among theorists and experimentalists. The working atmosphere within our department is dominated by an international flair bringing together young scientists from Brazil, Bulgaria, China, Egypt, France, Germany, India, Indonesia, Iran, Japan, Jordan, Korea, Russia, Spain, UK, and USA. This international orientation is also reflected by our main cooperation partners outside the Max-Planck-Society, i.e. RWTH Aachen (Prof. Bleck, Prof. Gottstein), University of Clausthal (Prof. Brokmeier), University of Göttingen (Dr. Klein), Carnegie Mellon University (Prof. Rollett), MIT (Prof. Radovitzky, Prof. Schuh), Technical University of Beijing (Prof. Mao), University of Lorena in Brazil (Prof. Sandim), and the National Institute for Materials Science in Japan (Prof. K. Hono).

The international visibility of the department is reflected by more than 50 keynote and invited lectures at international conferences in the past 6 years, numerous memberships of scientists from the department in international editorial, conference, and advisory boards, and a number of awards with which the department was honoured in the last 6 years. For instance Ms. Sc. Zaafarani, Dr. Singh, Dr. Zaefferer, Dr. Roters, and Prof. Raabe received the Best-Poster Award for their contribution “3D experimental investigation and crystal plasticity FEM simulation of the texture and microstructure below a nanoindent in a Cu-single crystal“ by the international committee of the 6th European Symposium on nano-mechanical Testing“ (Nanomech 6) in September 2005; Prof. Raabe was ranked 1st place of the TOP-10 list of the most important scientists in Germany below the age of 45 by the Journal “Bild der Wissenschaft” in June 2005; Ms. Sc. Takahashi was awarded the Friedrich-Wilhelm-Award of RWTH Aachen (Rheinisch-Westfälische Technische Hochschule Aachen) in December 2005; PD Dr. Winning received a Heisenberg-Scholarship of the Deutsche Forschungsgemeinschaft in January 2006; Dr. Konrad received the “First Price Niobium-Student Research Award” by the Institute of Materials, Minerals and Mining in May 2006; Dr. Ardehali Barani and Dr. Ponge received the “Stahlinnovationspreis 2006“ (Steel Innovation Award) for their work on high-strength spring steels (Entwicklung von hochfesten Stählen für Fahrwerksfedern) in June 2006; Dr. Zaefferer received the ThyssenKrupp Werkstoff-Innovationspreis 2006 in October 2006; Prof. Raabe was awarded with the ”Materials Science and Technology Price” of the Federation of European Materials Societies (FEMS) in Juni 2001; Dr. Zaefferer received the Masing award of DGM in 2001; Prof. Raabe received the “Dr. Meyer-Struckmann-Award

of the Brandenburgische Technische Universität Cottbus in Dezember 2001; Dr. Song, Dr. Ponge, and Prof. Raabe were awarded with the TMS 2004 Gold Medal Poster Award for the poster "Ultra fine grained steel after heavy warm deformation of ferritic-pearlitic C-Mn steels" at the TMS Annual Meeting 2004, Charlotte, USA in March 2004; Prof. Raabe received the Gottfried Wilhelm Leibniz Award of DFG in 2004. Furthermore, a number of visiting Professors and Humboldt fellows joint our group.

Selected Key Projects between 2001 and 2006

3D orientation electron microscopy by a joint focused ion beam-SEM-EBSD set-up

Zaefferer, Bastos, Zafaarani, Nellessen, Raabe

The department for microstructure physics and metal forming has in the past 2 years introduced the worldwide first fully automated 3D orientation electron microscopy technique. The method works via serial sectioning by using a Zeiss Crossbeam FIB-SEM instrument consisting of a focussed ion beam electron microscope in conjunction with an orientation imaging technique via EBSD (electron back scatter diffraction) in the SEM.

The system works reliably over long measurement times and produces very well aligned slices down to 50 nm distance. Combined with the maximum lateral resolution of EBSD which is in the order of 50 nm as well, it is possible to characterise volume pixels as small as 50×50×50 nm³. At maximum, volumes in the order of 50×50×50 µm³ can be examined.

The technique has been successfully applied for the study of the internal structure of pearlite, the crystallographic and morphological characterisation of fatigue cracks, the interface characterization in a NiCo-based microcrystalline electrodeposit material, the grain boundary characterization in FeSi alloys (Fig. 6), martensite investigation, and nanoindentation.

Consideration of geometrically necessary dislocations and of grain boundary mechanics in crystal plasticity finite element simulations

Roters, Ma, Raabe

Crystallographic slip, e.g. movement of dislocations on distinct slip planes is the main source of plastic deformation in most metals. The crystal plasticity FEM combines this basic process with the Finite Element Method by assuming that the plastic velocity gradient is composed of the shear contributions of all slip systems. Most crystal plasticity codes use empirical constitutive equations to describe these crystallographic shear rates. However, as crystal plasticity is build on dislocation motion and interaction, it is an obvious goal to introduce a constitutive model into such crystal plasticity FE codes which is based on dislocation densities as internal state variables. The dislocation model used in our new approach is based on six main ingredients: 1) For every slip system mobile and immobile dislocations are distinguished. 2) The immobile dislocations are grouped into parallel and forest dislocations for each slip system. 3) A scaling relation between mobile and immobile dislocations is derived. 4) The Orowan equation is used as kinetic equation. 5) Rate equations for the immobile dislocation densities are formulated based on distinct dislocation processes, e.g. lock formation or annihilation by dislocation climb. 6) Orientation

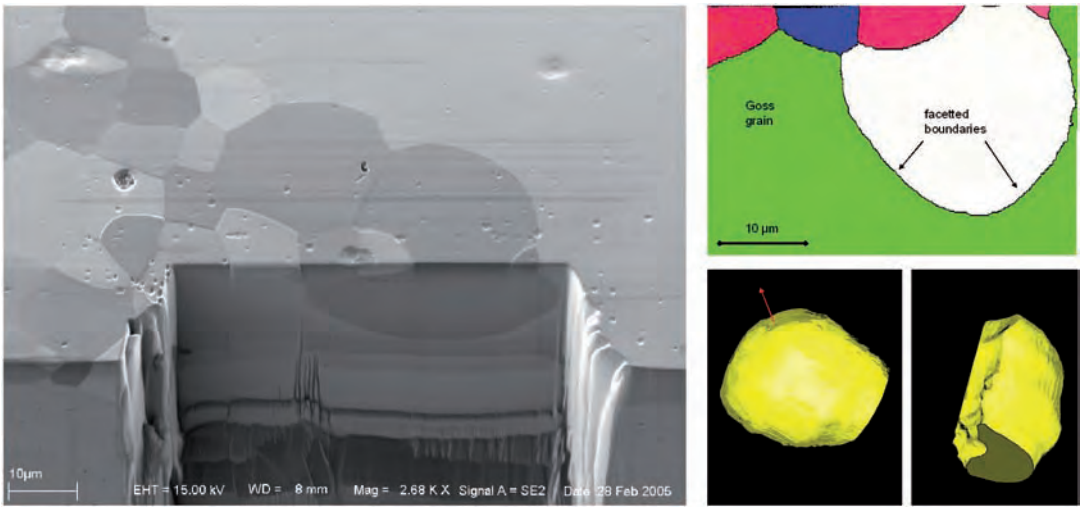

Fig. 6: *Grain boundary characterization in an FeSi alloy. The EBSD map on the right hand is coloured in terms of the crystallographic <hkl> vector. Many of such orientation slices have been combined to reveal the 3D structure of a grain (yellow images).*

gradients are implicitly described in terms of the dislocation density tensor. 7) We also introduce a physically based description of the mechanics of grain boundaries into the crystal plasticity FEM. While standard codes describe the grain boundaries as kinematical discontinuities (change of the orientation of the slip dyads between neighbouring Gauss points) the new approach introduces a physically based additional activation energy into the model in order to map the grain boundary resistance to slip penetration. Simulations on bicrystals with different orientation difference reveal excellent agreement with experiments both in terms of the texture and strain distribution [1-12].

Simulations and experiments on micro- and nanoindentation of metallic single crystals with and without polymer coatings

Zaafarani, Roters, Balasundaram, Nikolov, Raabe

This project is concerned with the simulation and experimental investigation of the mechanics associated with nanoindentation (Fig. 7) using high purity single crystals with and without polymer coatings. Experiments are conducted on a Hysitron nanoindentation set-up using a conical indenter in order to avoid symmetries others than those of the crystal structure. Orientation measurements are conducted using high resolution 2D and 3D EBSD techniques for texture mappings around the indents. Simulations are carried out by means of a 3D crystal plasticity finite element method which takes full account of crystallographic slip, orientation changes, and non-local gradient effects during the indentation [43]. The experiments and simulations are also conducted on polymer coated metallic single crystals in order to understand the micromechanics at the interface between the two phases.

Cellular automata for the simulation of recrystallization

Winning, Zambaldi, Brahme, Hantcherli, Raabe

Cellular automata are algorithms that describe the discrete spatial and temporal evolution of complex systems by applying local transformation rules to lattice cells which represent volume portions. The state of each site is characterized in terms of internal state variables. For recrystallization models these can be lattice defect quantities (stored energy), crystal orientation, or precipitation density. Each site assumes one out of a finite set of possible discrete states. The opening state of the automaton is defined by mapping the initial distribution of the values of the chosen state variables onto the lattice. The dynamical evolution of the automaton proceeds through the application of transformation rules (switching rules) that act on the state of each lattice point in discrete time steps. After each time interval the values of the state variables are updated for all points in synchrony mapping the new (or unchanged) values assigned to them through the transformation rule. Owing to these features, cellular automata provide a discrete method of simulating the evolution of complex dynamical systems which contain large numbers of similar components on the basis of their local interactions. The method is, like the related Potts Monte Carlo model, widely used in the department for applications in the field of recrystallization and recovery of steels and Al alloys. The transformation rules in such cases

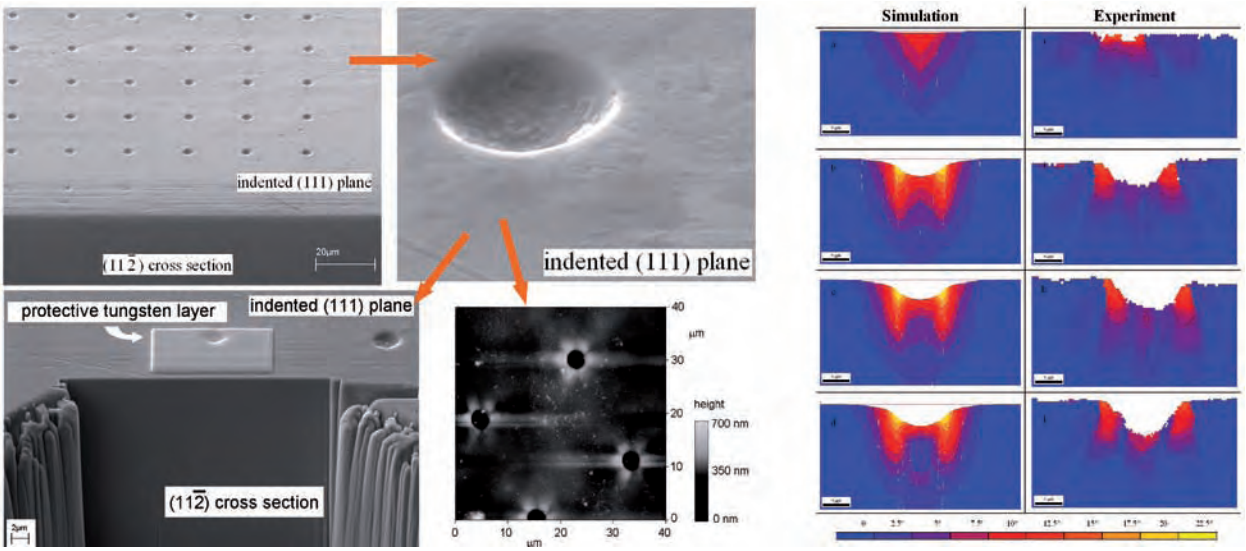

Fig. 7: *Left hand side: set-up of the 3D experiment for probing the crystallographic orientation beneath conical indents. Right hand side: set of four subsequent slices from an area outside of the conical indenter tip (top row) to areas close to the tip (bottom row). The left hand column shows viscoplastic crystal plasticity simulations. The left hand column shows the experiments. The colour code indicates the absolute magnitude of the orientation change relative to the original orientation of the Cu single crystal [43].*

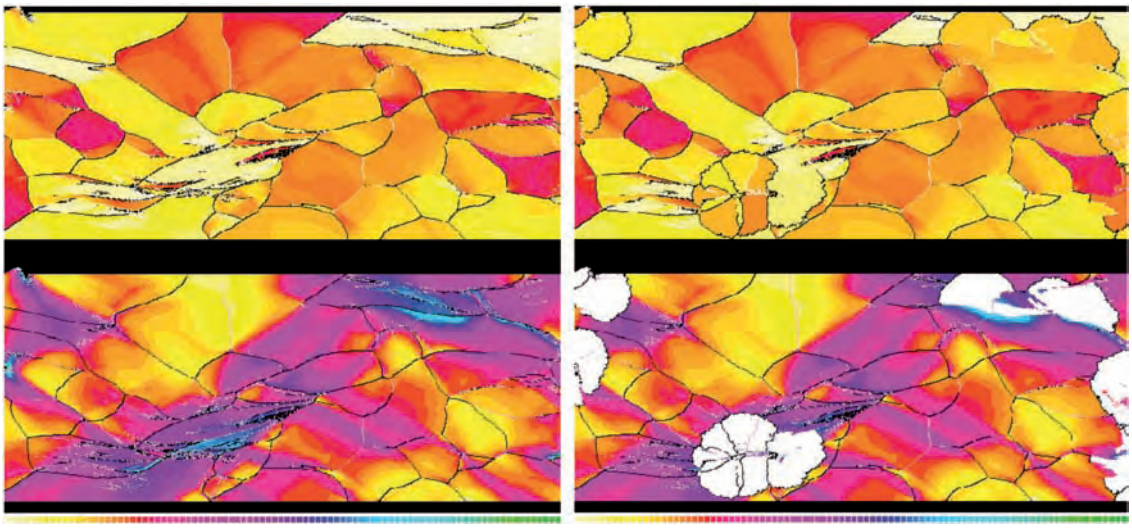

Fig. 8: *2D simulation of recrystallization in aluminium on the basis of crystal plasticity finite element starting data. Bottom: change in dislocation density; top: texture in terms of the magnitude of the Rodriguez vector. The white areas in the two bottom figures indicate a stored dislocation density of zero, i.e. these areas are recrystallized. Simulation parameters: 800 K; site-saturated spontaneous nucleation in cells with at least 50% of the maximum occurring dislocation density; growth misorientations above 15° at an activation energy of the grain boundary mobility of 1.46 eV and a pre-exponential factor of the grain boundary mobility of* $m_0 = 8.3 \times 10^{-3}$ $m^3/(N\,s)$.

reflect grain boundary rate equations and the stored energy is mapped in terms of appropriate dislocation density measures (Fig. 8) [44-49].

Grain boundary characterization in electro-deposited nickel-cobalt nanocrystals

Bastos, Zaefferer, Raabe, Schuh (MIT)

In this project we investigate nickel and nickel-cobalt samples with nano-sized grains produced by electrodeposition at MIT. The grain sizes of the specimens range from 40 nm to 800 nm in diameter. The grain boundary character distribution, the texture, and the micromechanics of such materials are investigated in detail by use of the 3D EBSD method (Fig. 9). The samples are also characterized by TEM. The nickel and nickel-cobalt samples show in the undeformed state a high fraction of first and higher order twin boundaries as well as elongated crystals which stem most likely from pronounced growth selection effects during the electrodeposition process [24].

Microstructure and texture of ultra fine grained C-Mn steels and their evolution during warm deformation and annealing

Ponge, Song, Torizuka, Murty, Zaefferer, Raabe

In this project we study the evolution of microstructure and texture of various C-Mn steels during large strain warm deformation and subsequent annealing. The process of grain subdivision during warm deformation is essential for the formation of ultra fine grains in such steels. Our work reveals that pronounced recovery instead of primary recrystallization is required to obtain a large fraction of high-angle grain boundaries as a prerequisite for the development of ultra fine grains during warm deformation. The prevalence of primary recrystallization instead of recovery is not generally beneficial since it reduces significantly the dislocation density and removes the substructure which is important for the gradual formation of subgrains and, finally, of ultra fine grains which are surrounded by high-angle grain boundaries. Consistently, the texture of ultra fine grained C-Mn steels observed after large strain warm

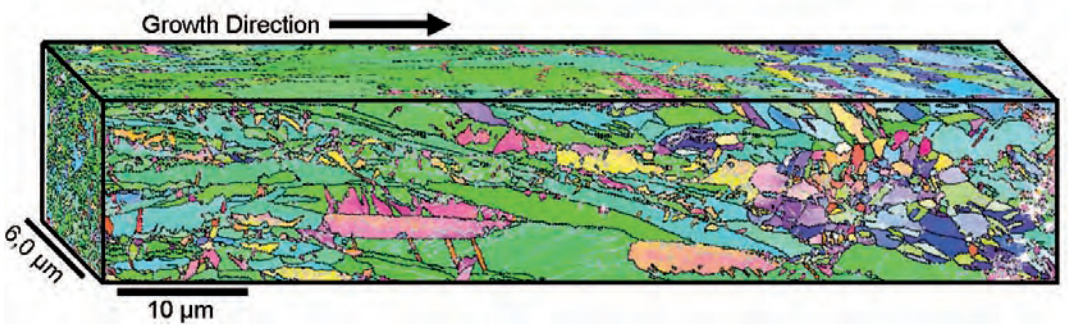

Fig. 9: *Worldwide first 3D view of a NiCo-based microcrystalline electrodeposited material as obtained by the 3D EBSD method.*

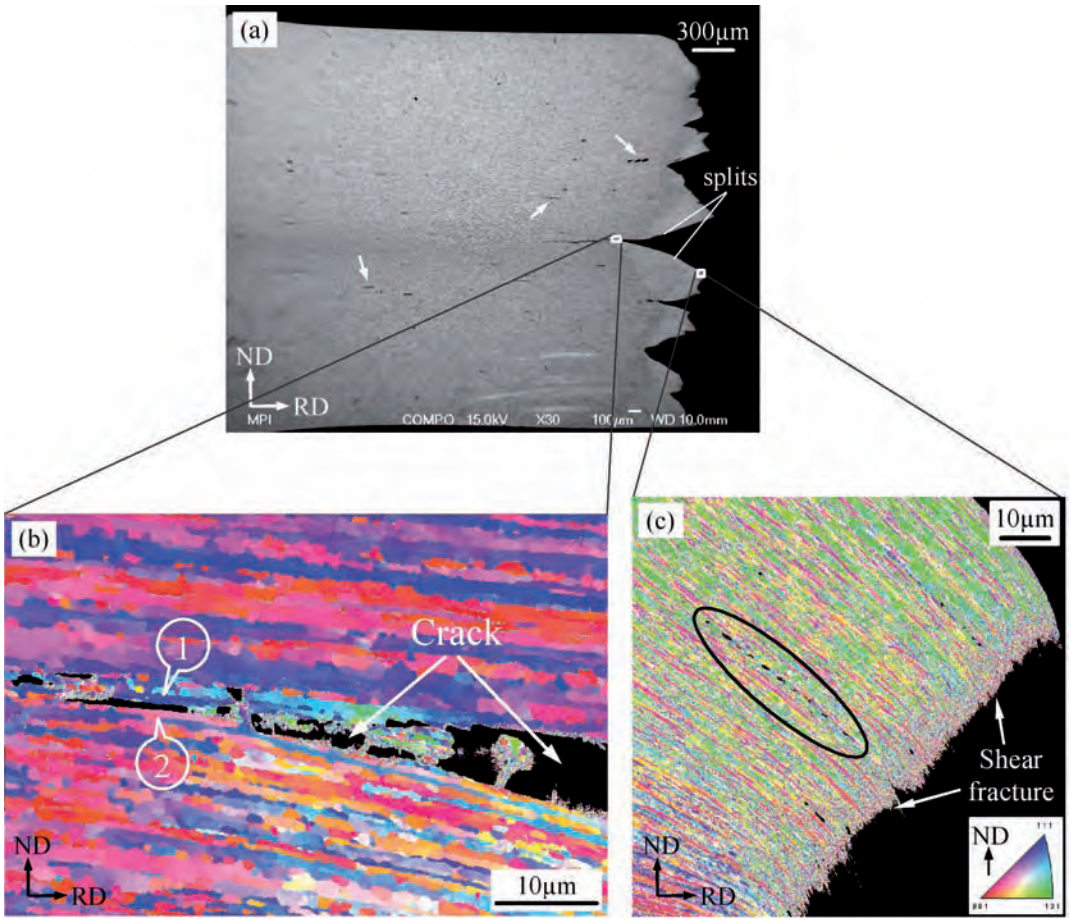

Fig. 10: *SEM image and orientation maps (taken by EBSD) of an ultrafine grained steel after a Charpy impact test conducted at 103 K. (a) Total view of the sample in transverse direction. The white arrows point out chains of large voids in the specimen. (b) Front of a crack. The circles 1 and 2 show two elongated grains with high–angle grain boundaries in between. (c) Aligned damage below a shear fracture. The ellipse highlights the alignment of voids along the grain boundaries. The orientation components in (b) and (c) are <111> || ND (blue), <001> || ND (red), and <101> || ND (green) [30-35].*

deformation and subsequent annealing, consists primarily of the <110> || RD texture fibre which indicates strong recovery. The <111> || ND texture fibre which is typical of recrystallized rolled ferritic steels does not appear. The process occurring during the deformation and subsequent annealing can, therefore, be interpreted as a pronounced recovery process during which new grains are created without preceding nucleation (Fig. 10) [30-35].

Texture and anisotropy in large scale crystal plasticity finite element simulations

Tikhovskiy, Roters, Eisenlohr, Raabe

The project is a numerical and experimental study on the influence of crystallographic texture on the earing behaviour in steels during cup drawing. The simulations are conducted by using different variants of the texture component or Fourier-based crystal plasticity finite element methods which account for the full elastic-plastic anisotropy of the material and for the explicit incorporation of texture including texture update. The methods are developed and improved in close cooperation with the German steel and automotive industry and in cooperation with the activities within the Max-Planck-Fraunhofer Initiative on Computational Mechanics of Polycrystals (Fig. 11).

Nano- and microscale fluid dynamics at rough interfaces

Varnik, Raabe

The aim of the project is a better understanding of fluid dynamics in the immediate vicinity of rough interfaces at the nano- and microscale. Particular aspects in this context are the transition from laminar to turbulent flow as a function of the roughness height and pattern of the interface and the mechanics in confined regions, such as occurring when fluids are trapped between two abutting rough metallic surfaces. The simulation tool for fluid dynamics at the nano- and microscale is a Boltzmann-lattice gas automaton [50-52].

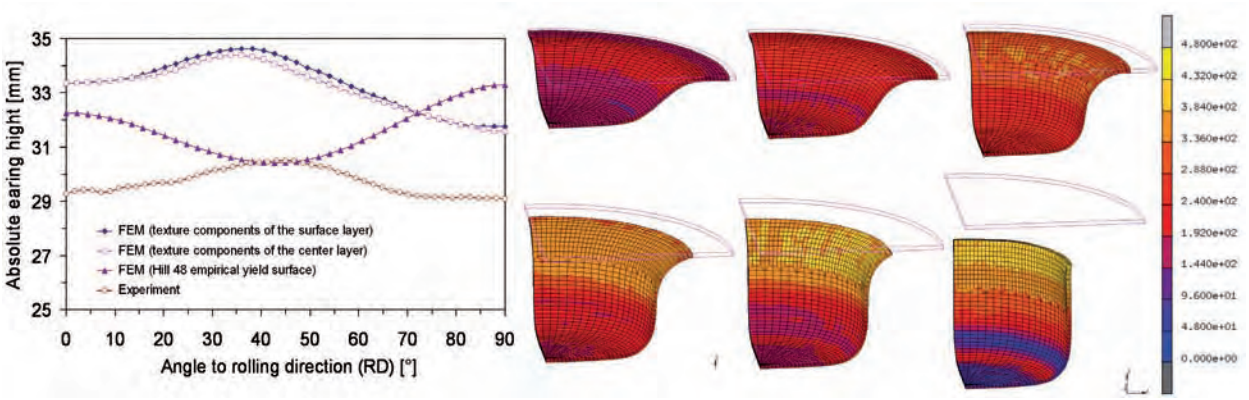

Fig. 11: *Simulations and experiment of earing during cup drawing of an aluminium alloy $AlMg_3$. Left hand side: The figure compares the texture component finite element simulation (TCCP-FEM) for texture components of the centre (s=0.0) and surface (s=1.0) layers with a simulation obtained by use of a Hill 1948 yield surface fitted on the basis of experimental r-values as typically used in industry. Right hand side: Some subsequent sketches of the simulation. The colour code indicates the von Mises stress.*

Effect of tramp elements in high strength SiCr spring steels

Barani, Ponge

This project deals with the optimization of the critical contents of trap elements in high strength spring steels through thermomechanical processing. It aims to minimize the negative effects of phosphorous, copper and tin on the final properties of springs used in the automotive industry. Depending on the concentration and the production process the aforementioned elements can cause two different problems, namely, the temper embrittlement and the liquid copper embrittlement. Within the framework of the project the rolling process and the heat treatment are simulated and the significant parameters are varied to improve the ductility and fatigue properties and maintain the required high strength level. The main interest is to avoid the above addressed embrittlement problems and to correlate the mechanical properties to the tramp element concentration and to the microstructure, i.e. to the austenite grain structure and the martensite morphology. Maximum concentration limits of the tramp elements will be deduced for different processing parameters. Apart from the standard production route the potential of the thermomechanical treatment will be investigated. The goal of the thermomechanical treatment is to achieve a better distribution of phosphorous through the conditioning of austenite in order to avoid its segregation to the grain boundaries (Fig. 12) [53-55].

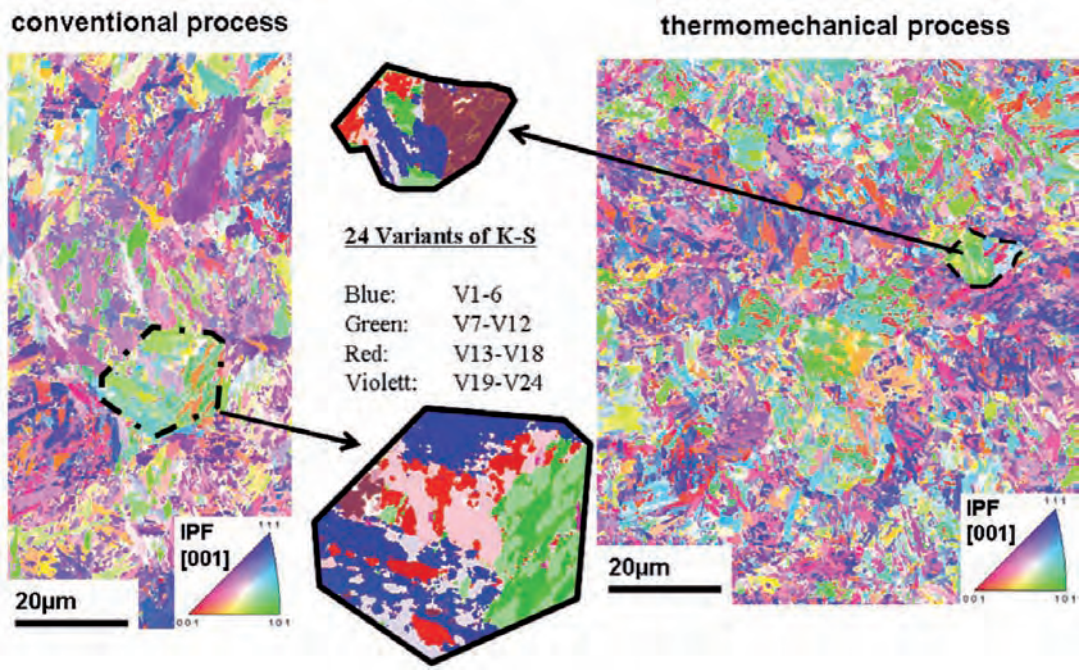

Fig. 12: *Microstructure results (EBSD) with a refined grain size obtained form an improved thermomechanical process (right hand side). K-S indicates variants of the Kurdjumov-Sachs crystallographic relationship [53-55].*

Heavy warm rolling for the production of thin hot strips with improved ductility

Ponge, Raabe

The project on heavy warm rolling for the production of thin hot strip aims to define processing parameters for rolling concept in which a hot strip coil produced on a conventional hot strip mill is to be transferred to a single high reduction rolling stand where a heavy warm reduction is imposed. For optimising the processing parameters the phase transformation behaviour is investigated for steels with 0.15, 0.35 and 0.67% carbon with and without austenite deformation at the previously optimized temperatures. After the optimum processing parameters the microstructure consists of spheroidised cementite, which is distributed homogeneously in a recrystallized ferrite matrix with fine grains [27-29].

Structure, texture, and mechanical properties of the cuticle of lobster

Sachs, Al-Sawalmih, Fabritius, Romano, Raue, Klein (Univ. Göttingen), Brokmeier (DESY), Raabe

The cuticle of lobster (homarus americanus) is a multilayer chitin-protein-based biological composite containing variable amounts of nanoscopic biominerals. Basically, the cuticle consists of three layers: Epicuticle, exocuticle and endocuticle. The epicuticle is an outer thin layer providing a permeability diffusion barrier. The exocuticle and endocuticle are made up of chitin fibres arranged in lamellas of different thickness. Local variations in composition and structure of the material provide a wide range of mechanical properties. It can be either rigid serving as a highly protective exoskeleton or it can be flexible serving as a constructional element as in articular membranes at joints. Consequently, the lobster cuticle is an excellent example of a highly versatile and efficient solution to structural and functional challenges for arthropods and probably also for comparable engineering challenges. In this Leibniz-project we conduct a systematic study on the correlation between the microscopic structure and the composition of the lobster cuticle on the one hand and the resulting local and global mechanical properties on the other. Many of the basic structural ingredients in such structures may at least in part occur in crystalline form (calcite, chitin). In that context we have observed for the first time that both, calcite and chitin are not at all distributed randomly in orientation space but they typically occur in a variety of preferred topological and crystallographic orientations. By use of X-ray wide angle analysis (synchrotron Bragg diffraction, laboratory-scale X-ray Bragg diffraction in conjunction with an area detector) we conduct corresponding texture investigations (Fig. 13) and correlate them with the observed microstructures which are characterized by TEM and SEM [38-42].

Development of novel beta-titanium alloys on the basis of first principles and experiments

Sander, Ma, Raabe, Friák, Neugebauer

In this project which is closely conducted together with the new department for Computational Materials Design we use a new strategy for the theory-guided bottom up design of beta-titanium alloys for bio-

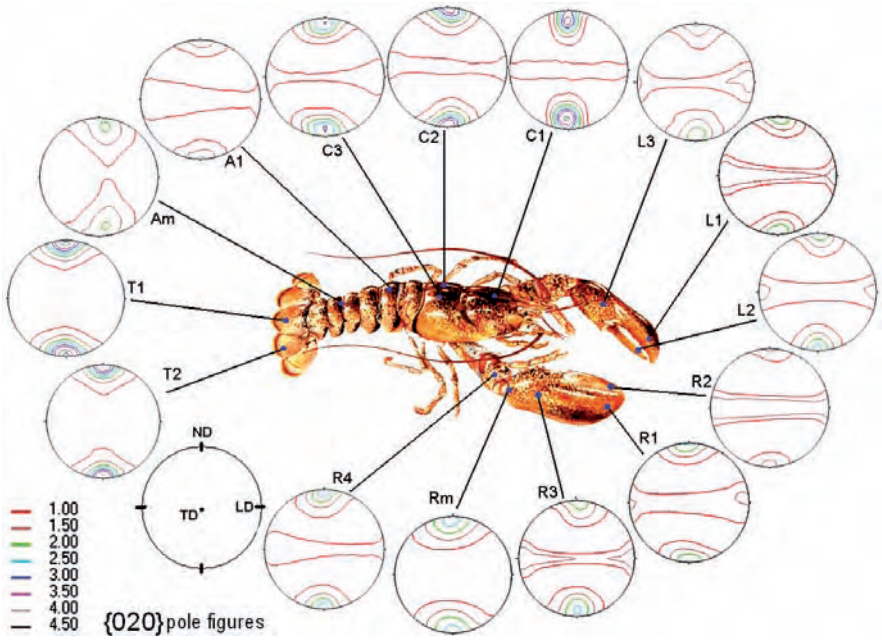

Fig. 13: *Survey of the {020} synchrotron pole figures of the orthorhombic α-chitin taken from different parts of the cuticle. LD : longitudinal reference direction; ND: reference direction normal to the local surface; TD: transverse direction. Regular sample numbering indicates that the specimens were taken from a highly mineralized part of the cuticle (L1, L2, L3, R1, R2, R3, R4, C1, C2, C3, A1). The annex m indicates that the sample was extracted from a soft membranous or respectively telson area (Am, Rm, T1m, T2m). L: positions on pincher claw, R: positions on crusher claw, C. positions on thorax, A: positions on abdomen, T: positions on telson.*

medical applications using a quantum mechanical approach in conjunction with experiments (Fig. 14). Parameter-free density functional theory calculations are used to provide theoretical guidance in selecting and optimizing titanium-based alloys with respect to three constraints: (i) the use of non-toxic alloy elements; (ii) the stabilization of the body centred cubic beta phase at room temperature; (iii) the reduction of the elastic stiffness compared to existing alloys. Following the theoretical predictions, the alloys are cast and characterized with respect to their structure, microstructure, texture, and elastic stiffness. Due to the complexity of the ab initio calculations, the simulations have been focused on a set of binary systems of titanium with different high melting bcc refractory transition metals such as Nb, Ta, and Mo. Various levels of approximations to describe mechanical and thermodynamic properties are tested and critically evaluated.

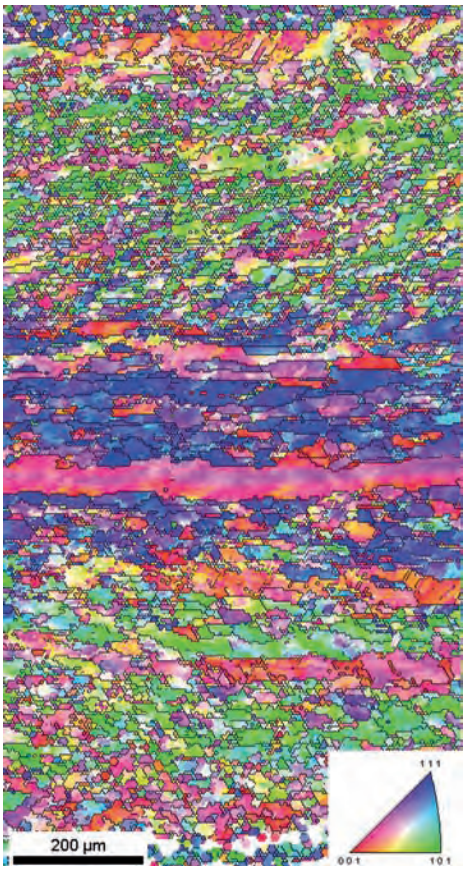

Fig. 14: *Longitudinal section (surface to surface) of a warm rolled Ti-35wt.%Nb-7 wt.%Zr-5 wt.%Ta alloy after 90% engineering thickness reduction. The specimen has a drastically reduced elastic stiffness when compared to conventional biomedical Ti-grades. It, hence, matches better the stiffness of bone and, thereby, could efficiently reduce mechanical shielding and resulting bone decay effects when used as an alloy for bioimplant applications.*

Texture and microstructure of TWIP steels

Raabe, Tikhovskiy, Ponge

The development of novel sheet steel grades for the automotive industry currently aims at increasing both, strength and formability with respect to applications in the field of optimal light-weight design engineering. High work hardening rates coupled with excellent internal damage tolerance mechanisms play an important role in the microstructure design currently pursued in that field.

In TWIP (twinning induced plasticity) steels the main mechanisms controlling the work hardening and the softening behaviour are related to a rather low stacking fault energy of the austenitic Fe-Mn-C phase. The stacking fault energy depends on the chemical composition and on the temperature. It governs the formation of twins, the double-cross-slip frequency of the dislocations, the frequency of the formation of certain sessile reaction products of the partial dislocations, and the recrystallization behaviour. In a set of new projects we currently investigate the effects of advanced hot rolling strategies on the resulting microstructures and textures of TWIP steels and their relationship with the observed mechanical properties (Fig. 15).

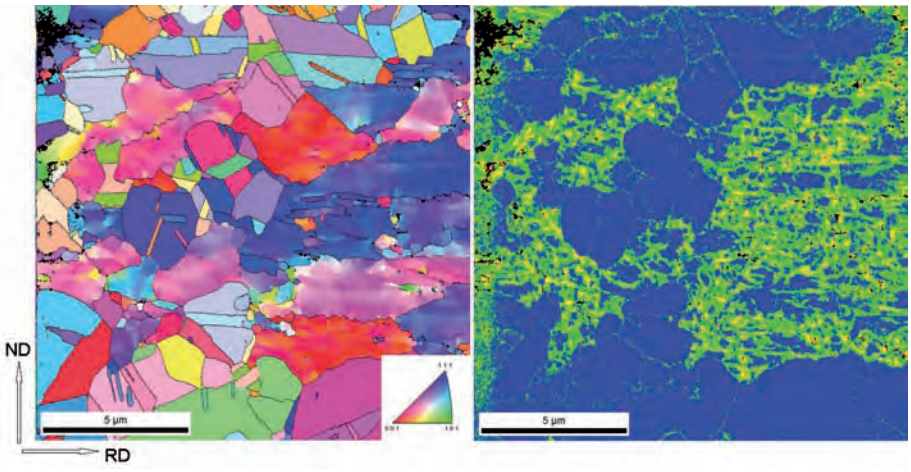

Fig. 15: *Left hand side: Microtexture of a warm rolled TWIP steel measured close to the hot band surface in the shear zone by high resolution EBSD. The colour code indicates the crystallographic <hkl> vector (see small standard triangle). Right hand side: Kernel average misorientation of the same region for separating the recrystallized regions (blue, low value) from the as-deformed regions (green and yellow, high value).*

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Research Projects in Progress

Theory and Simulation

Brahme, Winning, Raabe: Fast algorithms for physically-based recrystallization simulations in steels

Eisenlohr, Bieler (Michigan State Univ., USA), Roters, Raabe: Consideration of internal strain-induced damage nucleation phenomena in crystal plasticity finite element constitutive models

Eisenlohr, Roters, Van De Zwaag (Univ. Delft, NL) Raabe: Homogenization theory for multi-phase micromechanics constitutive laws in crystal plasticity finite element models

Friak, Ma, Sander, Neugebauer, Raabe: Combination of ab-initio simulations of lattice parameters, elastic properties, and phase stability and crystal plasticity finite element simulations for Ti-base alloys

Hantcherli, Eisenlohr, Roters, Raabe: Consideration of deformation-induced twinning in crystal plasticity finite element constitutive models

Nikolov, Balasundaraman, Meijer (Univ. Eindhoven, NL), Grundmeier, Raabe: Constitutive modeling of amorphous and of partially crystalline polymer mechanics with respect to indent and scratch phenomena in thin polymer layers

Petrov, Friak, Limperakis, Neugebauer, Sachs, Fabritius Raabe: Combination of ab-initio simulations and continuum models in biological materials

Raabe, Müller (MPI Leipzig), Roters: Modeling of deformation-induced patterning phenomena

Roters, Raabe: Dislocation density based and strain-gradient constitutive laws for crystal plasticity finite element simulations

Roters: Development of texture-function-based crystal plasticity finite element models

Tikhovskiy, Roters, Raabe: Crystal plasticity finite element simulations of deep drawing of stainless steels

Varnik, Raabe: Boltzmann lattice gas models for blood flow simulations

Varnik, Raabe: Simulation of scaling effects in nano- and microscale fluid dynamics at deformable metal surfaces

Varnik, Reuter (Fritz-Haber Inst.): Combined Boltzmann lattice gas and ab-initio models for modeling catalytic processes

Zaafarani, Roters, Larson (Oak Ridge Nat. Lab., USA), Raabe: Simulation of nanoindentation

Zaefferer: Monte Carlo Potts modeling for recrystallization nucleation and subgrain growth simulations

Zambaldi, Brahme, Raabe: Cellular automata for recrystallization simulation

Zambaldi, Roters: Crystal plasticity finite element simulations of plastic deformation of TiAl

Zhao (MIT, USA), Radovitzky (MIT, USA), Roters, Raabe: Massively parallel 3D crystal plasticity finite element simulations

Diffraction and Microscopy

Balasundaraman, Grundmeier, Nikolov, Raabe: Nanoindentation and nano-scratching in thin polymer layers

Bastos, Zaefferer, Schuh (MIT, USA), Raabe: 3D texture and microstructure analysis of electrodeposit Nickel-Cobalt nanocrystals

Frommert, Zaefferer, Günther(TKES, Gemany), Lahn (TKES, Gemany), Raabe: Secondary Goss grain growth in silicon steels

Kobayashi, Zaefferer, Ponge, Raabe: Microtexture and microstructure analysis in multiphase steels

Ma, Sander, Raabe: Microstructure, phase stability, and elastic properties of beta-Titanium alloys

Ponge, Murty, Raabe: Microtexture and microstructure of ultrafine grained steels

Romano, Friedel (TKS, Germany), Sommer (TKS, Germany), Zaefferer, Raabe: Microstructure of high-strength multiphase steels

Sandim (Univ. de Lorena), Bastos, Raabe: Microtexture in Niobium

Sato, *Zaefferer*: Investigation of orientation relationships in diffusional and martensitic phase transformations

Tao, Mao (TU Beijing), Raabe: Texture of diamond

Thiessen, Zaefferer, Imlau (RWTH Aachen, Gemany), Bleck (RWTH Aachen, Gemany): Texture and microstructure of multiphase steels

Yi, Zaefferer: Microscopic deformation mechanisms in Magnesium

Zaefferer, Kobayashi: Phase analysis for multiphase steels by use of a multiphase EBSD method applied to diffusion couple samples

Zaefferer, Zaafarani, Bastos, Raabe: 3D EBSD analysis by joint focused ion beam and electron back scatter diffraction microscopy

Metal Forming

Rasp, Yusupov: Continuum modeling of lateral flow and residual stresses in flat rolling

Thermomechanical Treatment

Ponge, Murty, Raabe: Processing and microstructure of ultra fine grained dual phase steels

Ponge, Raabe: Processing and microstructure of highly alloyed ferritic and austenitic stainless steels

Ponge, Raabe: Processing and microstructure of thermomechanically deformed TWIP steels

Torizuka (NIMS, Japan), Ponge, Raabe: Processing and microstructure of TRIP steels

Leibniz Group on Biological Nano-Composites

Al-Sawalmih, Fabritius, Raabe: Crystallographic texture of the cuticle of lobster and crab

Nikolov, Fabritius, Raabe: Constitutive micromechanical modeling of bone mechanics

Nyberg, Sachs, Fabritius, Raabe: Micromechanical properties of bone

Raabe, Klein (Univ. Göttingen, Germany), Raue, Fabritius, Brokmeier (DESY and Univ. Clausthal, Germany): Texture and smart anisotropy of biological nano-composites

Sachs, Fabritius, Raabe: Structure and micromechanical properties of the lobster cuticle

Others

Hono (NIMS, Japan), Raabe: Microstructure of wire drawn ternary high strength and high conducting Cu-base nanocomposites

PART III.

INTER-DEPARTMENTMENTAL RESEARCH ACTIVITIES - SELECTED HIGHLIGHTS

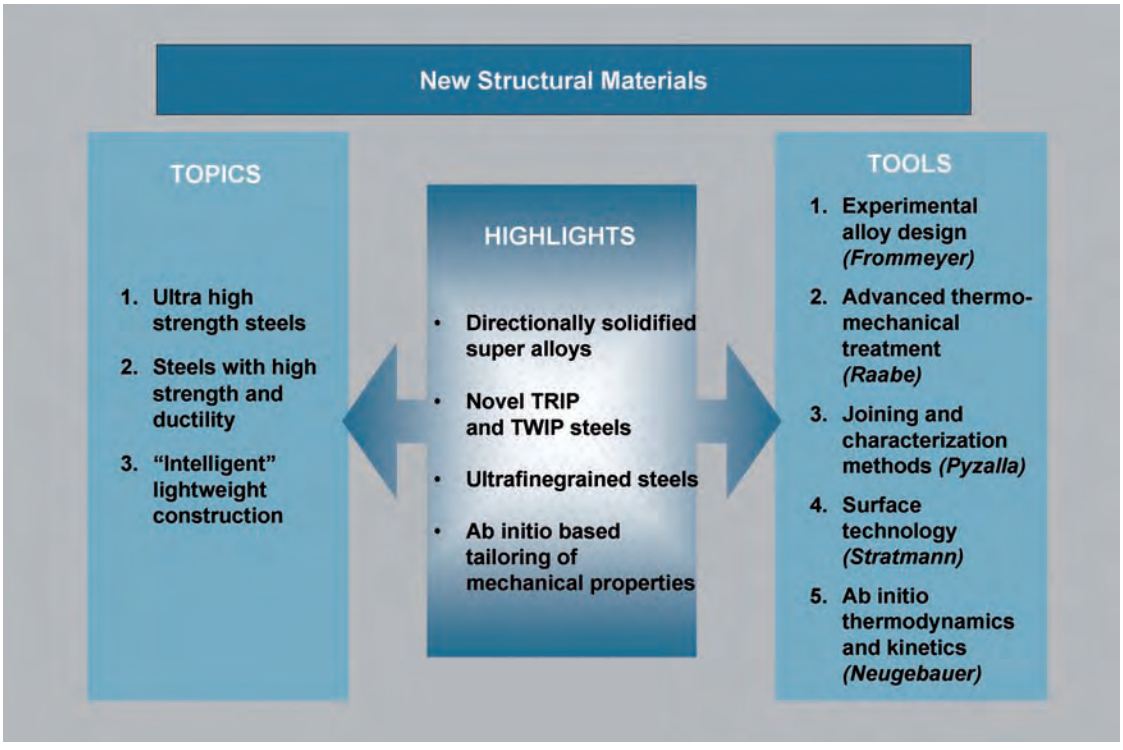
New Structural Materials

Introduction

The development and characterization of new structural materials is one of the major fields of activity of MPIE. Current research concentrates mainly on the development of new steels and innovative Fe-Al-base materials, on the characterization of new steels with complex microstructures, on thermo-mechanical processes as well as on understanding and preventing degradation processes in aggressive environments. All five departments are involved in this field, contributing with different tools: experimental alloy design (Frommeyer), innovative thermomechanical forming strategies and advanced characterization (Raabe), joining and characterization methods (Pyzalla), surface technology (Stratmann) and ab-initio modelling (Neugebauer).

The focus in the development of new steels is placed on new lightweight steels (Frommeyer). Ferritic high aluminium steels show potential for a pronounced reduction of the specific weight. Their cold forming limit could be widely expanded by micro alloying with B, Nb and Ti. Alloying with Al and Si also reduces the specific weight of TRIP and TWIP steels and allows adjusting the dominant deformation mechanism in these steels (transformation induced plasticity TRIP respectively twinning induced plasticity TWIP).These alloying concepts are combined in the development of DUPLEX and TRIPLEX steels based on the quaternary Fe-Mn-Al-C system (Frommeyer). Emphasis is further on the development of high strength steels; a recent highlight in this research area is the development of ultrahigh strength quasi-eutectoid steels. These modified pearlitic steels after severe drawing consist of extremely thin ferritic and cementite fibres and will presumably reach the theoretical strength of iron (Frommeyer, Rablbauer). In the new department 'Material Diagnostics and Steel Technology' (Pyzalla) activities have started to supplement the existing steel metallurgy by a powder metallurgy laboratory. Ongoing projects concern manufacturing of wear resistant steel MMCs by hot extrusion.

Laves phases form the largest group of intermetallic compounds. In steels Laves phases precipitates are used e.g. for increasing the creep resistance of martensitic/ferritic steels in power plants. A characteristic of Laves phases is their superior



high temperature strength which may lead to future functional and structural applications if their pronounced brittleness at ambient temperatures can be overcome. Several research projects in the departments 'Materials Technology' (Stein, Frommeyer) and 'Microstructure Physics and Metal Forming' (Raabe) in the framework of the inter-institutional research initiative 'The Nature of Laves Phases' of the MPG aim at a better understanding of the stability and changes in the polytypes of Laves phases and the resulting mechanical properties.

Research on innovative Fe-Al-based materials has been carried out as an inter-departmental research activity at MPIE over the last six years involving all departments. Considerable progress in the understanding of Fe-Al-based materials has been achieved, especially with regard to strengthening at high temperatures, the corrosion behaviour in various environments and in processing, particularly rolling (see short paper by Palm et al., p. 113). These advancements have led to a newly increased interest in Fe-Al-based materials worldwide, which is demonstrated by the fact that 75 participants from 12 countries attended the "3rd Discussion Meeting on the Development of Innovative Iron Aluminium Alloys - FeAl 2006" organised by the institute in January 2006. Also keynote lectures by members of the institute had been invited to open the sessions on Fe-Al-based materials at the EUROMAT 2005 and the 2006 MRS Fall Meeting. Furthermore the 2005 December issue of *Intermetallics* had been devoted to the Fe-Al activities at MPIE.

The Thermomechanical Processing group (Ponge, Raabe) aims at optimising steel for structural applications by controlling microstructure changes in deformation and annealing processes. Novel analytical developments in particular in the field of 2D and 3D EBSD techniques allow the characterization of microstructures of complex modern steels such as e.g. TWIP and ultrafine grained steels. For their achievements in optimizing the thermomechanical treatment of strong and ductile martensitic steels Ponge and Barani received in 2006 the prestigious steel innovation award in the category 'steel research and development' in the annual competition of the Stahl-Informationszentrum (steel information centre).

Understanding and preventing degradation processes of structural materials is one of the focal points of research in the department 'Interface Chemistry and Surface Engineering'. Special emphasis is on understanding the relationship between microstructure and reactivity. Reactivity is of particular importance in galvanizing processes for the new lightweight steels developed in the department 'Materials Technology'. The wetting behaviour of liquid zinc at partially oxidised surfaces is studied in the Molecular Structure Group (Rohwerder), high performance thermal pre-treatments on the basis of understanding thermodynamic and kinetic aspects on the selective surface oxidation of binary, ternary and quaternary model alloys (Swaminatham, Spiegel) are developed in the high temperature group (Spiegel).

Quantum mechanical based simulations by the Ab Initio Thermodynamic group have opened a novel way to understand, predict, and design alloy properties. In close connection with experiment the power of this approach has been demonstrated on two examples (Friak, Neugebauer, Raabe): (i) an investigation and interpretation of the volume-composition anomaly detected in Fe-Al alloys and (ii) identifying strategies to design biocompatible Ti-binaries for medical application. The first phenomenon is closely related to the above described development of new light-weight Fe-Al materials with optimized properties. The second topic aims at an improvement of hip transplants and addresses the lack of suitable materials which are biocompatible in terms of non-toxicity and mechanical properties matched to the bone.

High Carbon Steels of Quasi-Eutectoid Compositions Meet the Theoretical Strength of Iron

G. Frommeyer, R. Rablbauer

Department of Materials Technology

High carbon steels exhibit ultrahigh strength up to the theoretical limit when severely deformed to rods and wires. This results from the applied uniaxial deformation by wire drawing introducing high dislocation densities in the coexisting ferrite and cementite lamellae appearing as extremely thin fibres of about 50 nm in diameter or less. Therefore a considerable contribution by fibre reinforcement of the constituents will also strongly increase the strength. In quasi-eutectoid and hypereutectoid pearlitic steels the yield and ultimate tensile strengths are primarily dependent on the pearlite colony size, interlamellar spacings, and mean lamellae thickness quantified by the relationship: $\sigma_y = \sigma_0^* + k s^{-1/2}$. This expression is similar to the Hall-Petch equation where σ_0^* is the Peierls stress - intrinsic friction stress of the crystal lattice - governed by the cementite constituent of the pearlite with large interlamellar spacings of $s \cong 10$ μm. The coefficient k represents the slope of the σ_0^* vs. f $s^{-1/2}$ plot. It has been found not to be sensitive to temperature, composition, and strain rate [1]. The interlamellar spacing is decreasing with increasing amount of undercooling ΔT. The cooperative growth theory of pearlitic transformation yields a relation between the spacing *s* and undercooling ΔT as

$$s \propto \frac{\gamma \cdot T_e}{\Delta H_e \, \Delta T}$$

where γ, T_e, and ΔH_e represent the ferrite/cementite interfacial energy, the eutectoid temperature, and the transformation enthalpy [2].

Solid solution hardening of the α ferrite and cementite phases due to alloying additions, such as C, Cr, Si, Al and thermomechanical processing procedures like patenting for achieving ultrahigh strength and retaining sufficient ductility of the thin wires have to be taken into account. These factors will effect the microstructural features, like volume fractions of the ferrite/cementite constituents, and the misfit between the ferrite/cementite lamellae or fibres in the heavily deformed state.

The primary approach for achieving high strength of tire cord is to increase incrementally the carbon content. The tensile strength of high carbon steel is shown in Fig. 1.

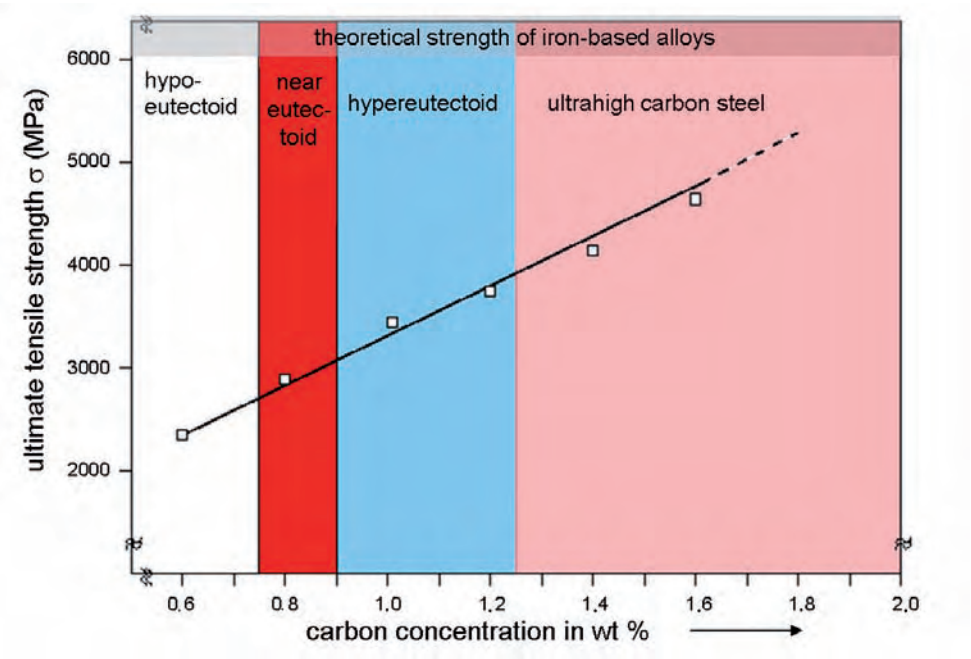


Fig. 1: *Ultimate tensile strength of highly deformed carbon steel wires as a function of carbon content, degree of deformation* $\eta = 99$ *%.*

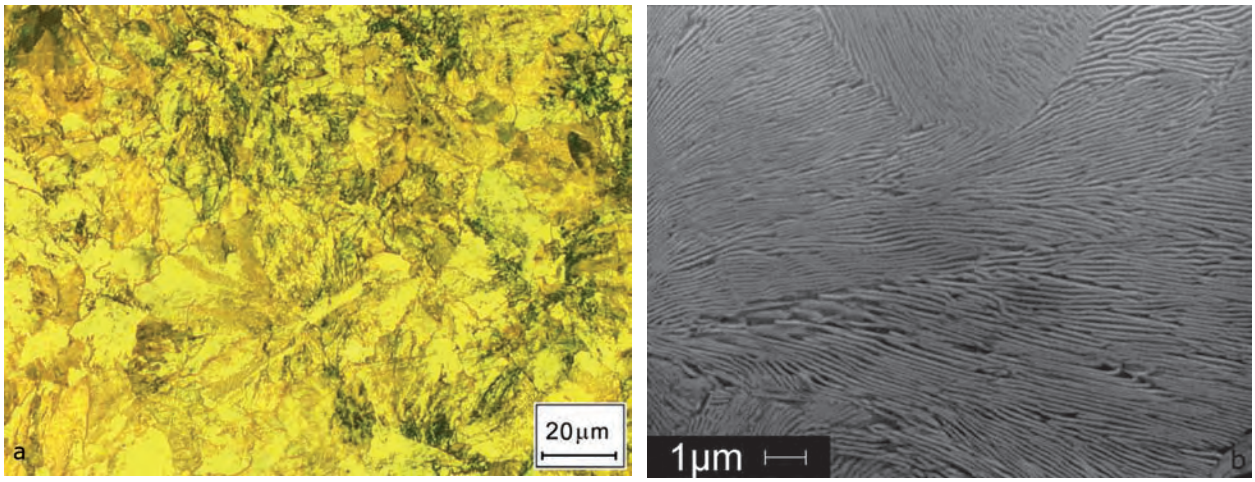


Fig. 2: *Light optical (a) and SEM (b) micrographs exhibit a very fine pearlite microstructure of a modified Fe-1.25C-(Al, Cr) steel.*

The diagram represents the general tendency of the tensile strength as a function of the carbon content in mass % for a wire deformed with a reduction of cross section of about η = 99 % . Conventional premium tires possess eutectoid or slightly hypereutectoid carbon steel cord exhibiting a strength of about 3400 to 3600 MPa [3]. The projected strength for ultrahigh carbon steels with carbon contents of 1.25 % to 1.4 % reaches strength levels of 3850 to 4200 MPa [4], respectively. However, it should be noted that in hypereutectoid steels the proeutectoid cementite formed along primary austenite grain boundaries or around pearlite colonies will reduce the amount of cold deformation by breaking up the cementite lamellae or fibers. However, the formation of undesirable proeutectoid carbide networks can be controlled by phase transformations and thermomechanical processing. Alloying additions that were found to inhibit the formation of cementite networks include Si and Co. The application of higher cooling rates in the patenting process is also of great importance to prevent the formation of proeutectoid cementite. Higher cooling rates suppress the formation of proeutectoid cementite during the austenite to pearlite transformation. For example, by applying a cooling rate of dT/dt = 10^2 K/s a hypereutectic carbon steel with c_c = 1.3_5 mass % will not form a cementite network. From the diagram it can be seen that heavily drawn steel wires with carbon contents of about 1 mass % may achieve a strength level of about 3300 MPa. For fine cord of d = 80 µm in diameter and higher degree of cold deformation tensile strength values of 4500 MPa will be achieved [2].

Small amounts of chromium of about 0.5 mass% and 0.1 mass % vanadium should be added to the carbon steels in order to refine the transformed pearlitic microstructure, as shown in the optical and SEM micrographs of Fig. 2a. In addition finely dispersed vanadium carbides will increase the strength by precipitation hardening.

The optical and SEM micrographs are revealing a very fine-grained pearlite structure with interlamellar spacings of less than 0.1 µm [5,6]. By adding certain amounts of aluminum to the hypereutectic steels the formation of proeutectoid carbide can be prevented and the strength will increase due to very effective solid solution hardening of the α-ferrite and markedly reduced interlamellar spacings or extremely thin α-Fe and Fe_3C fibers to nano-size dimensions.

Fig. 3 represents the ultimate tensile strength of ultrahigh strength quasi-eutectoid steels of the composition Fe-1.25C-(Cr,Al) severely deformed by wire drawing to a superpearlitic fine cord in comparison to pearlitic piano wires (Fe 0.85 % C) and technically pure iron possessing about 0.01 mass % carbon as a function of reduction of cross section 'η' or logarithmic degree of deformation 'φ'. From the figure it can be clearly seen the quasi-eutectoid pearlitic steel exhibits a considerable increase in strength up to 6000 MPa at the highest degree of deformation due to the in-situ formation of nano fibers of the coexisting phases possessing an average fiber diameter of 20 nm [5]. The pearlitic piano wires exhibits strength values greater than 4000 MPa, respectively. The equations inserted in the drawing describe the strength in dependence on the shear moduli, the Burgers vector and the reciprocal square root of interlamellar distances. The achieved strength maximum of 6000 MPa is comparable with the theoretical shear strength of b.c.c. iron.

The first well-known estimations of the theoretical values for shear and tensile strengths are

$$\tau_{theo}^{Fe} = \frac{G|\vec{b}|}{2\pi \cdot h}$$ [7] and $$\sigma_{theo}^{Fe} = \left(\frac{E\gamma}{a_0}\right)^{\frac{1}{2}}$$ [8], where

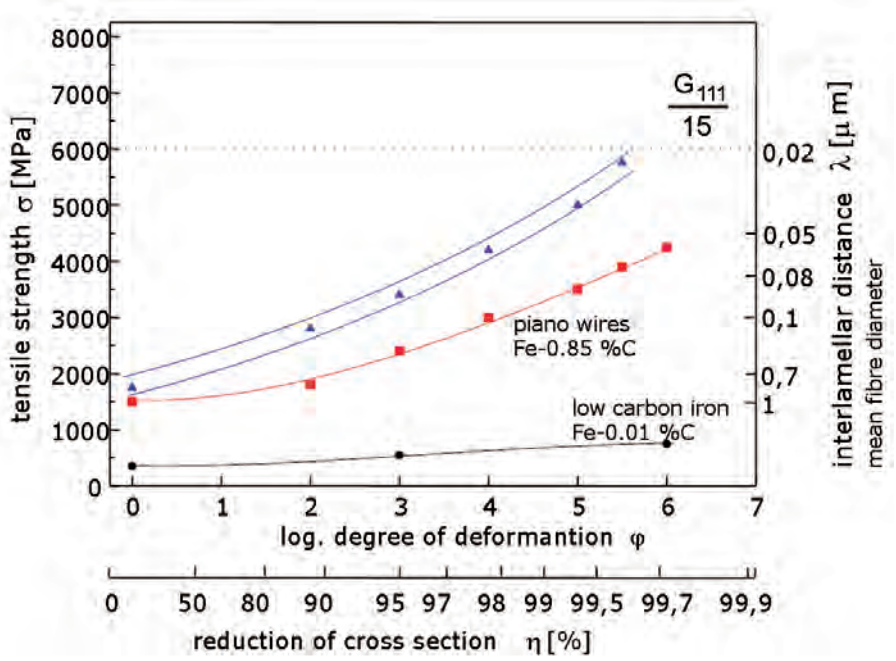


Fig. 3: *Ultimate tensile strength in dependence on logarithmic degree of deformation and reduction of cross section.*

G = 83 GPa and E = 216 GPa [9] are the elastic shear and Young's moduli for iron, $\vec{b}$ is the Burgers vector, h is the distance of the consecutive shear planes, γ represents the surface energy and a_0 is the lattice constant. Theoretical shear strength of $\tau^{Fe}_{theo} \approx G/2\pi \approx 13$ GPa was estimated for b.c.c. iron. In the classical work of Brenner [10] a maximum tensile strength of $\sigma_{111} = 13.4$ GPa was recorded in miniaturized tensile tests on whiskers of few micrometers in diameter. However, the following aspects have to be considered. The whisker was orientated and tested along the hard [111] crystal orientation. The given value was found exclusively for whisker diameters of $d \cong 2$ µm, respectively. Whiskers of non determined orientations and of similar sizes of $d \geq 3$ µm in diameter did not exceed in general the tensile strength of $\sigma = 5.5$ GPa. A theoretical shear strength of $\tau^{Fe}_{theo} \approx G/15 \approx 6$ GPa has been established in the literature [11] arguing that the theoretical tensile strength would be higher by considering the Taylor factor in confidence with the experimental results by Brenner. When evaluating the theoretical strength in greater detail the crystal anisotropy has to be considered. For different crystal orientations the Young's moduli of α-iron are given as follows: $E_{100} = 134$ GPa, $E_{110} = 223$ GPa, and $E_{111} = 285$ GPa [12]. Recently performed ab initio calculations of the cohesive strength of iron evaluated values of $\sigma_{th} = 12.7$ GPa for the [100] and 27.3 GPa for the [111] crystal orientations [13]. These calculated values fit with the experimental results regarding the fact that not the theoretical (cohesive) tensile strength but the shear strength will represent the limitation for maximum stresses in experiment.

The TEM micrograph of Fig. 4 exhibits the microstructure of a severely drawn pearlitic wire after a degree of cold deformation of = 99.5 % revealing whisker-like ferrite and Fe_3C fibers of nano-size diameter of about 20 nm. In comparison to the single-crystalline whiskers grown and investigated by Brenner the diameter of these structures are about 100 times smaller. Although severely drawn pearlitic wires exhibit a sharp [110] texture as common for b.c.c. metals, however, for polycrystalline material, even under ideal uniaxial tensile test condition, the crack initiation in the zone with the highest deformation will always be promoted by the shear stresses of the weak [100] crystal orientation. Con-

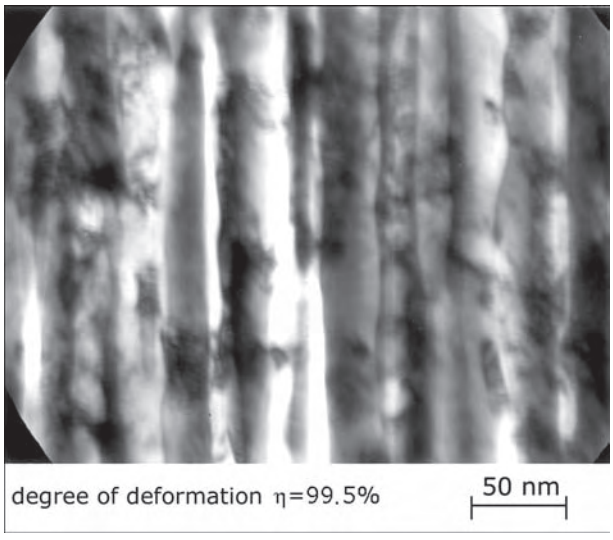


Fig. 4: *TEM bright-field image showing nano-sized cementite and ferrite fibers of the quasi eutectoid ultrahigh carbon fine cord. Large fiber areas appear free of dislocations.*

sidering the different materials conditions it can be concluded that Brenner's single crystal whiskers as well as severely drawn modified pearlitic steels consisting of extremely thin ferrite and cementite fibres meet the theoretical strength of iron.

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Steel MMCs by Powder Hot Extrusion

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Lifetime of many components, in particular of tools is limited by abrasive wear. An efficient way of increasing wear resistance is the reinforcement of metallic matrices with coarse hard phases, usually carbides (WC, NbC, TiC), nitrides or borides. These particle reinforced metal matrix composites cannot be manufactured by conventional metallurgy, they are usually deposited e.g. on steel substrates by a HIP-cladding process. In the HIP-cladding process, however expensive near-net-shape capsules are needed. As an alternative to HIP-cladding we pursued the idea to produce steel MMC profiles via hot extrusion of pre-sintered powder capsules.

We chose a common cold work tool steel X220CrVMo13-4 and a common hot work tool steel X40CrMoV5-1 as steel matrices. Both tool steels were reinforced with up to 30% coarse WSC (monolithic WC+W_2C) respectively TiC (agglomerated) particles.

The Fe-base MMCs were hot extruded on the 8MN horizontal press at the Extrusion Research and Development Center of the Institute of Material Science and Technology of TU Berlin. In order to reduce the force during the hot extrusion process the encapsulated powders (powder can diameter 78mm) were sintered at 1150°C for 2h. The green bodies after sintering show open porosity, their density is about 0.5. The powder cans were hot extruded at 1150°C (extrusion ratio 5.2:1, stem speed: 35 mm/s, temperature of stem and container: 480°C, lubricant: glass). The density of the hot extruded products was at least 97.5%. All products were free of surface defects (Fig.2).

Microstructure analyses of the hot extruded MMCs revealed no significant defects within the profiles. The long axis of the monolithic WSC hard phases appears to be re-oriented towards the longitudinal direction of the profiles by the hot extrusion process. Texture

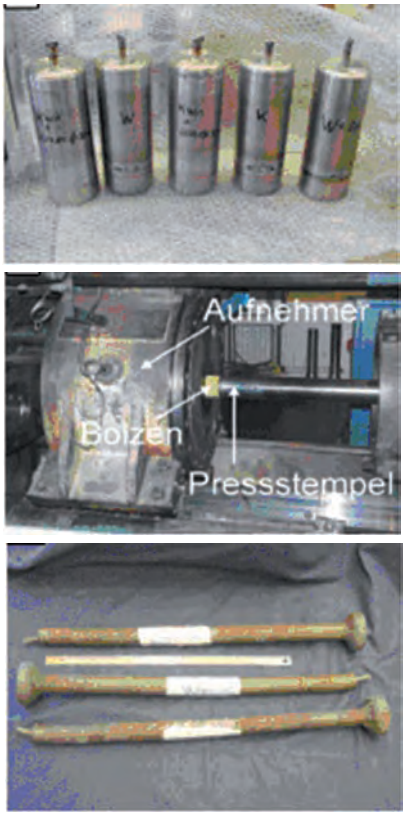

Fig.1: *Powder cans, hot extrusion press at TU Berlin, hot extruded profiles.*

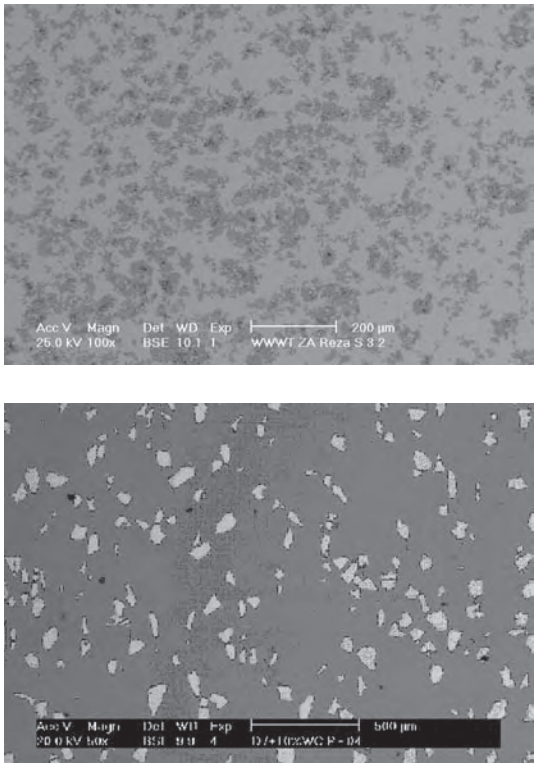

Fig. 2: *Microstructure of extrudates: Top: X220CrVMo13-4 + 30% TiC, bottom: X220CrVMo13-4 +10% WSC*

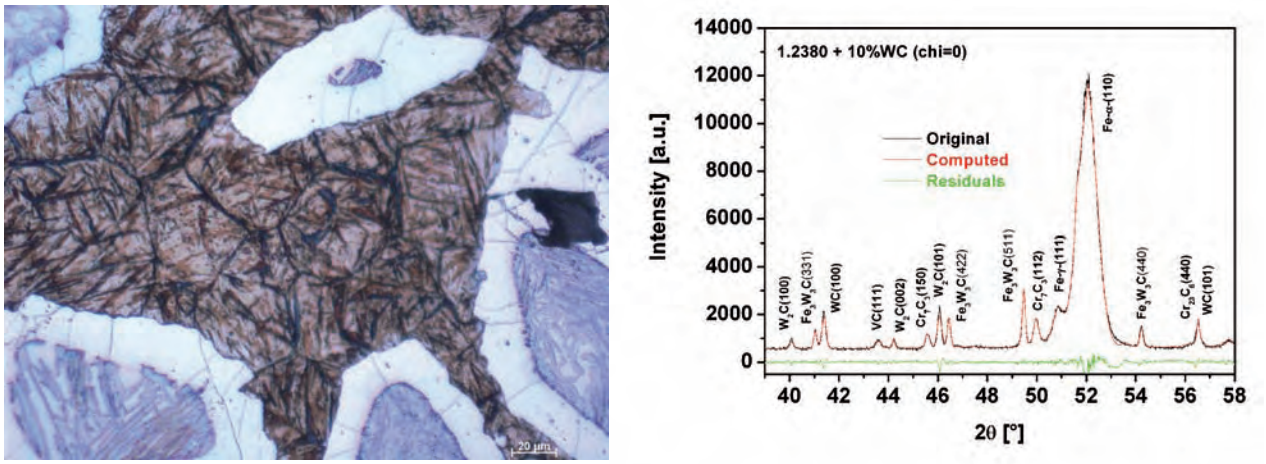

Fig. 3: *Microstructure of X40CrMoV5-1+30%WSC: Left: Optical microscopy showing the η-carbide seam around the WSC and retained austenite in the steel matrix; right: Synchrotron X-ray diffractogram, phase identification by Rietveld refinement.*

analyses also revealed a preferred <0001>-direction of WSC in extrusion direction.

In hot extruded MMCs with high hard phase volume fractions hard phase clusters are visible, which are extended in extrusion direction. Material flow during the hot extrusion process, in particular friction between the extrudate and the die results in hard phase agglomeration in the near-surface region of the extrudates.

Interdiffusion during sintering and hot extrusion result in V enrichment of the TiC particles, further bonding between the TiC hard phases and the steel matrix does not occur. In contrast interdiffusion between the WC and the steel matrix results in the formation of η-carbides seams around the WC. These η-carbides are brittle and often contain cracks in radial direction due to stresses encountered during the hot extrusion process as well as due to thermal residual stresses formed during cooling because of the thermal expansion mismatch between the carbides and the steel. The volume fraction of η-carbides however was smaller than in comparable HIP-products. The hot extrusion process has only minor influence on the chromium carbide distribution and volume fraction in the steel matrix, but, due to carbon diffusion from the coarse hard phases into the steel matrix during sintering and hot extrusion high retained austenite volume fractions are present in the steel matrix (Fig.3).

In order to optimise the wear resistance of the hot extrusion products the MMCs were subjected to a further heat treatment consisting of hardening and annealing. Pin-on-disc tests of the hot work tool steel matrix materials against SiC abrasive showed an increase of wear resistance of the WSC reinforced MMCs while the wear rate of the TiC reinforced MMCs was comparable to those of the steel matrix. In case of the smoother SiO_2 abrasive the pin-on-disc tests even revealed an increase in wear resistance of up to two orders of magnitude of the 30% WSC particle reinforced hot work steel when compared to the pure steel matrix.

Innovative Fe-Al-Based Materials

M. Palm [1], A. Schneider [1], F. Stein [1], G. Sauthoff [2], M. Friák [3], S. Zaefferer [4], L. Agudo [5], A.R. Pyzalla [5], M. Spiegel [6]

[1] Department of Materials Technology, [2] Department of Physical Metallurgy, [3] Department of Computational Materials Design, [4] Department of Microstructure Physics and Metal Forming, [5] Department of Material Diagnostics and Steel Technology, [6]Department of Interface Chemistry and Surface Engineering

The development of Fe-Al-based materials for structural applications is focussed on optimisation of strength, creep and corrosion resistance at high temperatures and sufficient ductility at lower temperatures. In order to achieve this ambitious aim investigations on the constitution, microstructure, mechanical properties, and high-temperature corrosion behaviour of Fe-Al-based materials with Al contents ranging from 10 to 45 at. % have been carried out within an inter-departmental research activity in all departments at MPIE.

Phase diagram studies, modelling and diffusion. The binary Fe-Al system has been reinvestigated by differential thermal analysis (DTA) [1]. While the basic features of the phase diagram have been confirmed, the liquidus and solidus temperatures have been thoroughly determined for the first time (Fig. 1). Within the framework of the COST action 535 "Thermodynamics of alloyed alumindes - THALU" phase equilibria in the Fe-Al-Ni [2] and the Fe-Al-Ti [3] systems, which both are core systems for the development of Fe-Al-based materials, have been assessed. Also phase equilibria in the Fe-Al-Ti-Cr-C system have been experimentally investigated with emphasis on the precipitation kinetics of the phase TiC from the melt [4]. A TTT diagram for the precipitation of TiC in the α phase is shown in Fig. 2. In an Fe_3Al-Cr-Mo-C alloy the sequence of carbide precipitation in the temperature range 700–1000 °C has been studied by high resolution scanning electron microscopy (HRSEM) where phases were identified by electron backscattering diffraction (EBSD) and their compositions were established by energy dispersive spectrometry (EDS) [5].

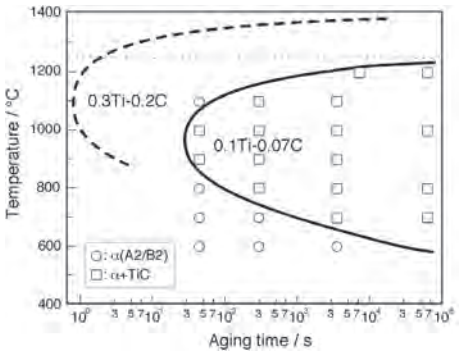

Fig. 2: *TTT diagram for the precipitation of TiC in the α-Fe(Al) phase.*

Atomistic ab initio studies demonstrated that the origin of the experimentally observed anomalous composition-volume dependence in FeAl alloys is due to a magneto-volume instability [6]. Anelastic

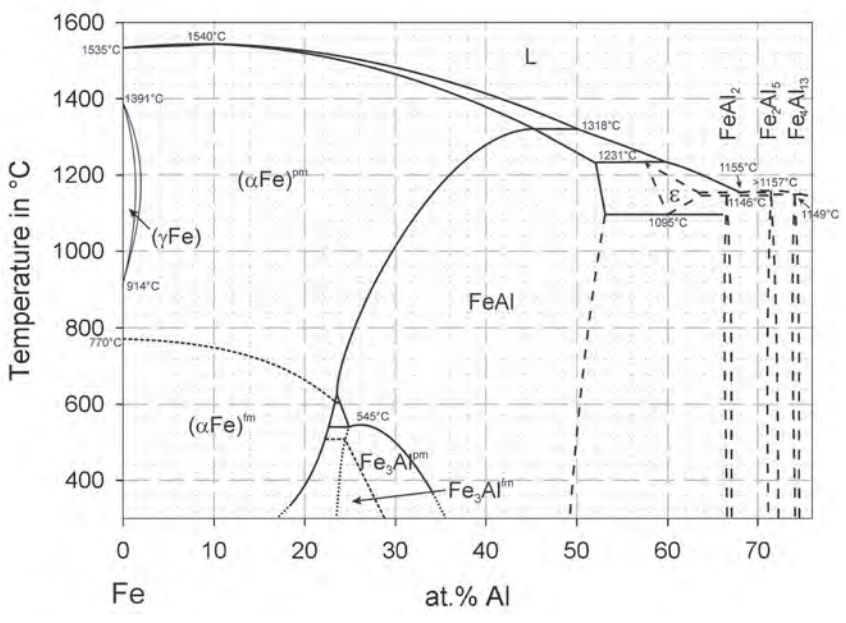

Fig. 1: *Fe-Al phase diagram reinvestigated by DTA.*

relaxation effects caused by vacancies and C atoms in Fe-Al-(Ti, Nb) were investigated by mechanical spectroscopy, positron annihilation spectroscopy and by radio tracer diffusion [7]. From these studies vacancy concentrations in dependence on temperature – which have a marked influence on mechanical properties –, diffusion rates and the activation enthalpy for the removal of carbon atoms from the solid solution have been determined.

Microstructure/mechanical properties relations. A large number of projects have been devoted to the processing of differing microstructures and their effects on the resulting mechanical properties. The effect of incoherent precipitates of carbides [8,9], borides [10] and various intermetallic phases [11-13] have been studied. Accordingly also the effects of coherent precipitates [14] and of increased ordering of the Fe-Al matrix [12,13] have been studied and the achievements of the different concepts have been analysed in detail [15,16]. Fig. 3 gives an overview on the gain in creep strength that has been obtained by the different strengthening concepts. The comparison with P92 – an advanced martensitic/ferritic Fe-9 wt.% Cr steel for power plant applications – shows that the newly developed Fe-Al-based materials partly show a much higher creep resistances.

Like for other high-strength materials for use at elevated and high temperatures the limited ductility up to ambient temperatures is also a concern for Fe-Al-based materials. In order to gain a fundamental understanding of the ductility of Fe-Al-based materials the brittle-to-ductile transition temperature (BDTT) of binary Fe-Al has been established as a function of the Al content [17]. Between 0 - 40 at.% Al the BDTT increases slightly from –100 to about 100 °C before it "jumps" up to about 800 °C at Al contents exceeding 40 at.% Al. The "jump" is accompanied by a change in the fracture mode from transgranular below 39.6 at.% Al to intergranular above 41.3 at.% Al with mixed mode fracture in the small composition range in between. In contrast to the binary alloys rather high BDTTs are generally observed for ternary and higher order alloys [11,12,14] with the notable exceptions of Fe-Al-C and Fe-Al-B-based alloys [8,10]. In order to comprehend the large difference in BDTT between binary and higher order alloys a systematic study on the BDTT of ternary Fe-Al-X alloys has been started [18].

Improved ductility and toughness may also be achieved by grain refinement. For Fe_3Al-based alloys a thermo-mechanical process has been established by which fine-grained microstructures can be obtained [19-21]. For a hot-rolled material this thermo-mechanical process consisted of a heat treatment at 1100 °C for 10 min, by which a grain refinement and dissolution of large carbide particles has been achieved, followed by compressive deformation during the subsequent rapid cooling.

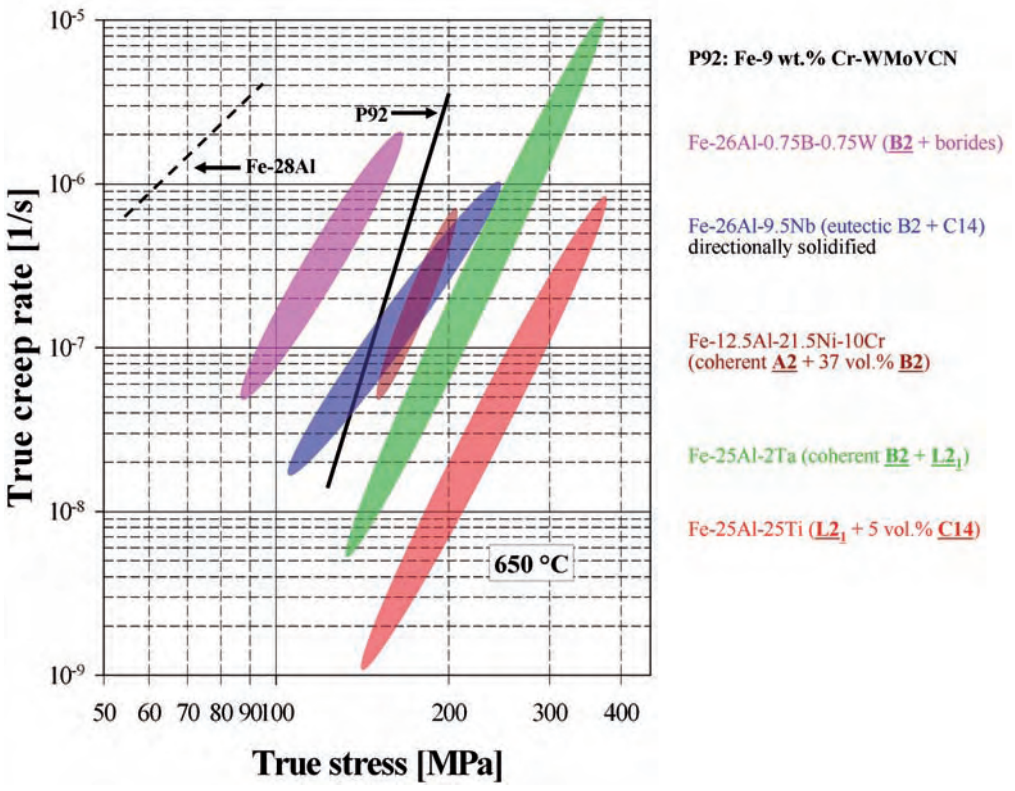

Fig. 3: *Creep strength of various Fe-Al-X alloys in comparison with the Fe-9 wt.% Cr steel P92.*

Processing, machining and joining. For the production of components rolling, machining and joining are essential processes which have to be well understood. To elucidate the parameters for hot rolling, a Fe-26 at.% Al alloy has been investigated by means of the hot deformation simulator (WUMSI) [22, 23]. With the obtained process parameters hot rolling was then performed in the disordered (A2) as well as the B2-ordered regime and the resulting differences in the microstructures were carefully analysed which led to the optimisation of the thermo-mechanical treatment. By a combined approach by three-dimensional EBSD with a focussed ion beam (FIB) technique orientation gradients around a hard Laves phase particle in a warm-rolled Fe_3Al-based alloy have been investigated [24] (Fig. 4).

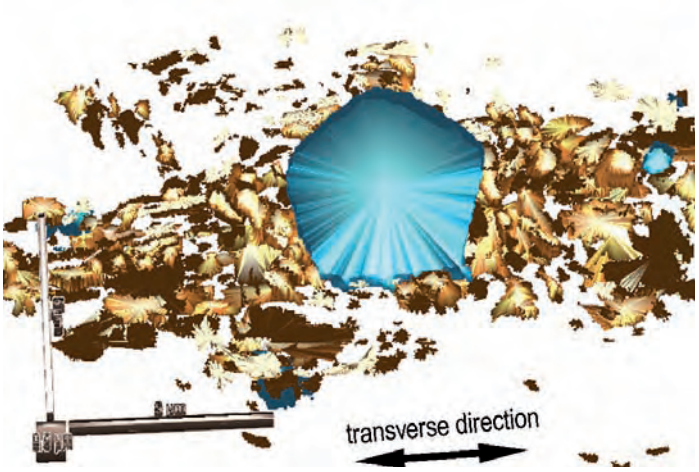

Fig. 4: *3D visualisation of areas of low local misorientation in the vicinity of a hard Laves phase particle in a warm-rolled Fe_3Al-based alloy. The Laves phase is coloured blue. The areas which are characterised by a weak average local misorientation of less than 2.5° are coloured gold.*

In a joint project together with the Institute of Production Engineering and Machine Tools, University Hannover, the machinability of Fe_3Al-based alloys is currently investigated [25]. Tool wear and chip formation in dependence of cutting speed, feed, depth and tool material are studied.

Iron aluminide formation in steel/Al joints is a major factor determining their strength and ductility. In a joint project with voestalpine Stahl GmbH and Fronius International GmbH the formation of Fe_xAl_y-intermetallic phases, their dependence on filler composition in CMT ("cold metal transfer" by Fronius International GmbH) metal arc welding and the influence of the intermetallic phase seam on the weld mechanical properties was studied [26].

Corrosion behaviour. As the excellent corrosion behaviour is one of the outstanding properties of Fe-Al-based materials, corrosion is studied in various hostile environments. The oxidation behaviour has been studied for binary [27] and ternary alloys [11,12,16]. Special emphasis has been put forward to the understanding of the formation of protective oxide layers by studying the early stages of their formation by combined X-ray photoelectron spectroscopy (XPS), grazing incidence XRD with synchrotron radiation and transmission electron microscopy (TEM) [27]. For Fe-15 at.% Al and Fe-40 at.% Al no difference in the oxide growth mechanisms up to 300 min could be determined. After 5 min a double oxide layer consisting of Al_2O_3 and Fe_2O_3 is observed (Fig. 5) whose development was studied in dependence on temperature and exposure time. Below this double oxide layer at the interface to the iron aluminide, an epitaxially formed, metastable Al_2O_3 layer, most likely consisting of Θ-Al_2O_3 or γ-Al_2O_3, was found.

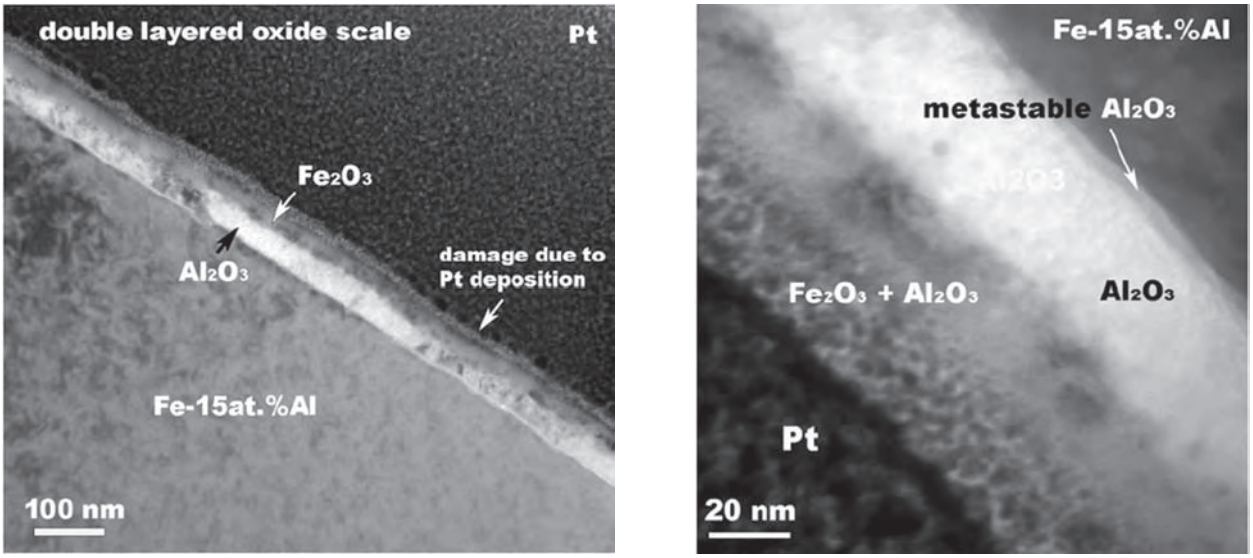

Fig. 5: *TEM high-resolution bright field images of a double oxide layer consisting of Al_2O_3 and Fe_2O_3 formed on Fe-15 at.% Al after oxidation at 700 °C for 300 min.*

The hot corrosion resistance in NaCl-KCl melts, which is a major concern for waste incinerators and biomass-fired boilers, has been evaluated for a number of model alloys [28]. While Cr has a detrimental effect on corrosion in Fe-Cr alloys under such conditions, Al shows a beneficial effect by improving the corrosion resistance. Metal dusting is another high temperature corrosion process which leads to the degradation of iron, low-alloyed and high-alloyed steels as well as Ni-base and Co-base alloys in strongly carburising atmospheres. The investigation of metal dusting of binary Fe-Al alloys with Al contents ranging between 15 and 40 at.% Al in strongly carburising CO-H_2-H_2O gas mixtures at 600 °C revealed that also for metal dusting an increasing Al content slows down the carburisation reaction [29]. The details of the metal dusting process have been studied for Fe-15at.% Al [30]. While cementite (Fe_3C) was only observed in the coke – which is the reaction product of the metal dusting – oriented needle-like or plate-like precipitates of κ-phase (Fe_3AlC_x) were found in the Fe-Al matrix close to the surface and their orientation relationship with the matrix was established employing EBSD.

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Optimized Thermomechanical Treatment for Strong and Ductile Martensitic Steels

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Department of Microstructure Physics and Metal Forming

Nowadays, quenched and tempered, medium carbon martensitic steels are widely used for applications where high mechanical strength is the main design driver. But besides strength in most engineering applications a good ductility, toughness or fatigue and corrosion behaviour are demanded. To obtain a good compromise between strength and toughness the as quenched martensite is reheated to temperatures between 150 and 700°C to obtain the required level of toughness without a significant loss in strength. With decreasing tempering temperature the strength increases while the ductility or toughness decreases. Thus higher strength levels can not be achieved by conventional heat treatment methods that only offer a few possibilities to design the material properties. Additionally, most commercial steels contain impurities that influence the toughness and ductility significantly. The well known embrittlement phenomenon observed around 350°C is such an example where grain boundary segregation of impurity elements together with carbide films at grain boundaries deteriorate the mechanical properties of the material [1-5].

Martensite forms by a displacive transformation from the parent austenite phase. Therefore, the grain and dislocation structure, or in general the defect structure of the austenite is inherited to the product phase, because the relationship between neighbouring atoms does not change. Thus the microstructure of the austenite is very crucial for the final properties of the martensite. Research at our Institute has shown that austenite deformation prior to quenching can lead to an increase in strength without adverse effects on ductility or toughness. For a medium carbon chromium vanadium steel Peters and Wettlaufer demonstrated [6-9] that by deforming the austenite, its grain size and grain substructure can be controlled in such a way to produce high strength martensitic steels with excellent ductility, toughness and endurance limit.

The silicon chromium steel 54SiCr6 (Fe-0.54C-1.4Si-0.65Cr-0.65Mn (mass%)) was selected for our investigations. Since the early 90ies most of the automotive coil springs in Europe are made of this steel grade. It exhibits high strength and good sag resistance [12-13]. To study the sensibility to harmful elements the content of phosphorous (0.0023 to 0.0213 mass %), of copper (0.169 to 0.540 mass %), and of tin (0.0193 to 0.060 mass %) was systematically varied. The ratio of tin to copper was always kept constant at 0.1. The experimental alloys used were prepared from high-purity base materials as 70kg vacuum induction melts. Bars were rolled after annealing at 1100°C for heat treatment and thermomechanical treatment experiments. All the treatments were carried out using the large scale 2.5MN hot press at Max-Planck-Institut für Eisenforschung [14-15].

It was reported earlier that the maximum in strength and ductility of martensite is achieved when prior to quenching the austenite is deformed around 900°C with a strain slightly below the peak strain [16]. To understand the effect of a recrystallised or a non-recrystallised microstructure on the mechanical properties including the effect of the impurity elements, we kept the deformation strain (0.4) and rate (5/s) constant and varied the deformation temperature. The microstructure was observed after quenching.

Fig. 1 summarizes the results for the conventional heat treatment (CHT). The well-known dependence of ductility and strength on tempering temperature was observed. Additionally the effect of the impurity elements was determined for various tempering

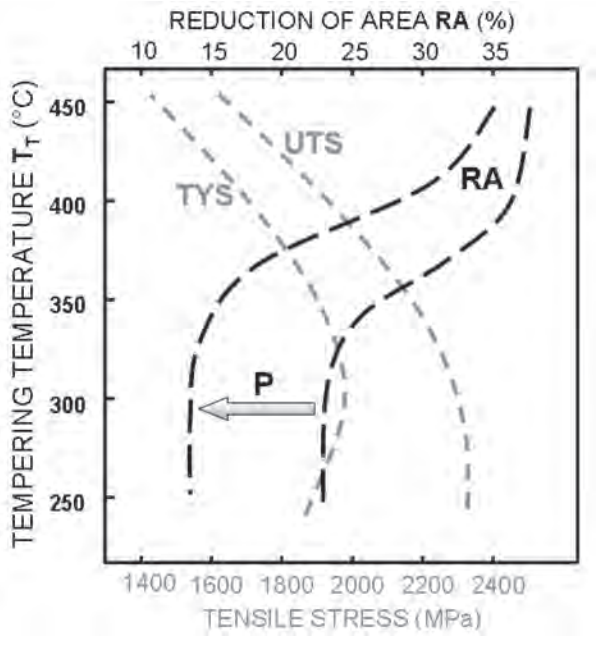

Fig. 1: *Tensile properties of quenched and tempered 55SiCr6.*

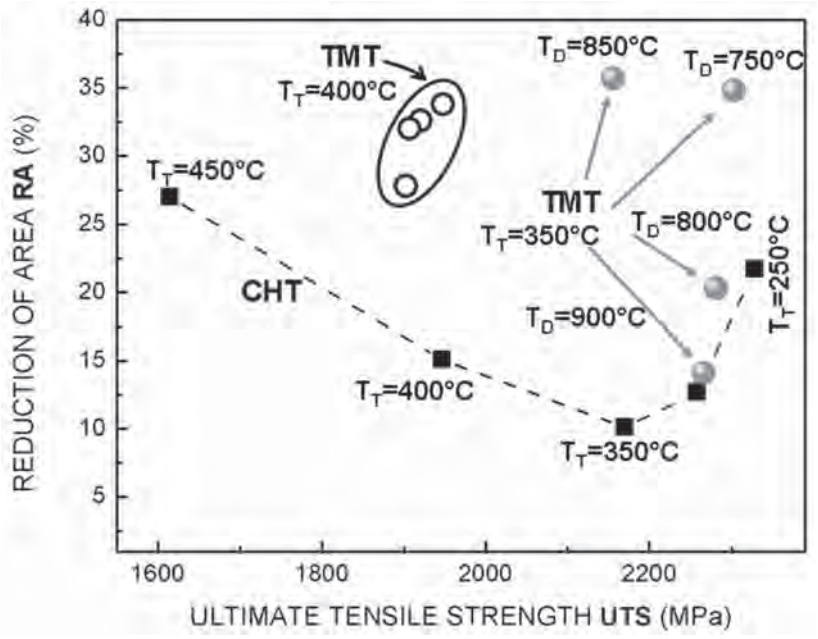

Fig. 2: *Combination of strength and ductility for 55SiCr6 with 0.54 Cu and 0.054 Sn (mass %), T_T: tempering temperature, T_D: deformation temperature.*

temperatures and processes. A strong reduction of the ductility is caused by addition of phosphorus or the addition of copper and tin.

In Fig. 2 the combination of ductility and strength is shown for the melt with the highest copper and tin concentration. The reduction of area of conventionally heat treated samples is relatively low at all tempering temperatures and only after tempering at 450°C it reaches values above 25 %. To ascertain the effect of the austenite microstructure and condition on the resulting mechanical properties samples were deformed at various temperatures prior to quenching and tempered at 350 and 400°C. All deformed samples (TMT) exhibit a higher ductility than the conventionally heat treated samples tempered at the same temperatures. A deformation can improve the ductility above the value obtained after conventional heat treatment and tempering at 450°C. Fig. 3 compares the fracture surfaces of a conventionally heat treated sample tempered at 350°C with a thermomechanically treated sample tempered at the same temperature. The first sample fails in an intergranular brittle way while the second shows no sign of embrittlement. As we have shown [17] the deformation of the austenite can refine or eliminate the formation of carbide films at prior austenite grain boundaries (Fig. 4).

Two austenite conditions, a recrystallised and a non recrystallised condition corresponding to deformations at 850 and 750°C respectively, were selected for further investigation. Samples were austenitized at temperatures between 900 and 1000°C and then deformed at the aforementioned temperatures to produce the two austenite conditions. The mechanical properties of these samples after tempering at 300°C are compared for the steel with the highest phosphorous concentration (Fig. 5). Independent of austenitization temperature, the

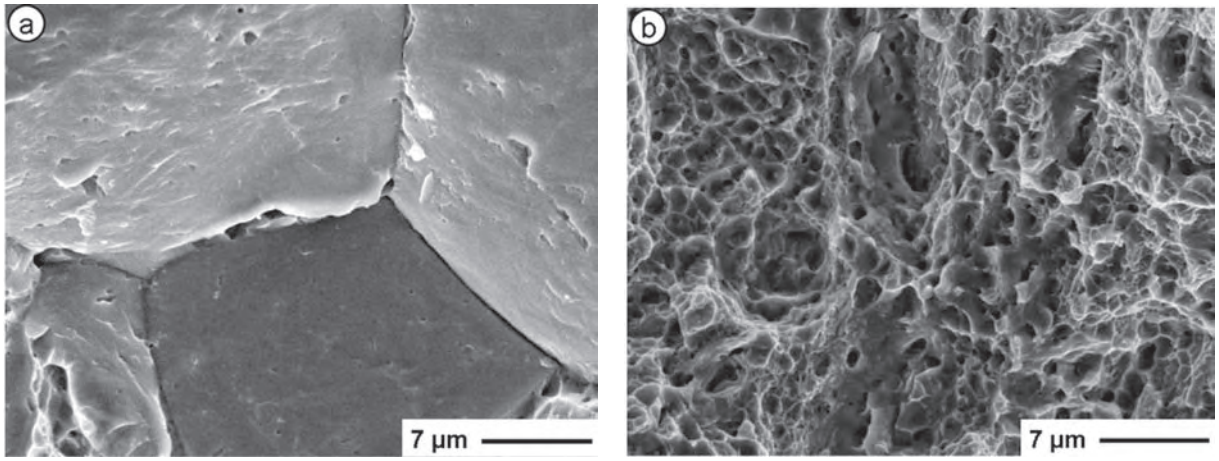

Fig. 3: *Scanning electron micrographs of fracture surfaces of 55SiCr6 samples with 0.54Cu and 0.054 Sn (mass %) tempered at 350°C: a) conventional heat treatment, b) thermomechanical treatment.*

reduction of area of the TMT samples is at least three times higher than after conventional heat treatment. The reduction of area of the recrystallised austenite modification (TMT_{RX}) is independent of austenitization temperature. After deformation at 850°C the austenite recrystallises and grain refinement occurs. Independent of austenitization temperature the recrystallisation after deformation at 850°C led always to a similar austenitic grain size. The reduction of area of the non-recrystallised austenite modification (TMT_{NRX}) increases with decreasing austenitization temperature. The austenite grain size is dependent on the austenitization temperature. The deformation only elongates the austenite grains and produces a work-hardened austenite. It does not refine the grain size. From the observations an optimized thermomechanical treatment was tested for the entire composition range: A first deformation is carried out at 850°C to refine the austenite grains followed by a second deformation at 750°C to produce the desired work-hardened defect structure. The enhancement of ductility for the same strength level (above 2200 MPa), i.e. same tempering temperature (300°C) is presented in Fig. 6. This two-step thermomechanical treatment delivers mechanical properties that are not sensitive to impurity element content (within the range tested) [18].

Applying a deformation prior to quenching improves the mechanical properties of quenched and tempered martensitic steels. The austenite microstructure prior to quenching has a strong influence upon the size distribution of the martensitic units (i.e. packets, blocks, lath) [19], the dispersion of carbides during tempering, and the carbide morphology at the prior austenite grain boundaries. Furthermore, the microstructure can be tailored in such a way to minimize the sensitivity to embrittlement by reducing the segregation driving force or by maximizing the grain boundary area, and by doing so decreasing the grain boundary concentration of the impurity elements. Thereby, a significant improvement of both strength and ductility is possible at the same time.

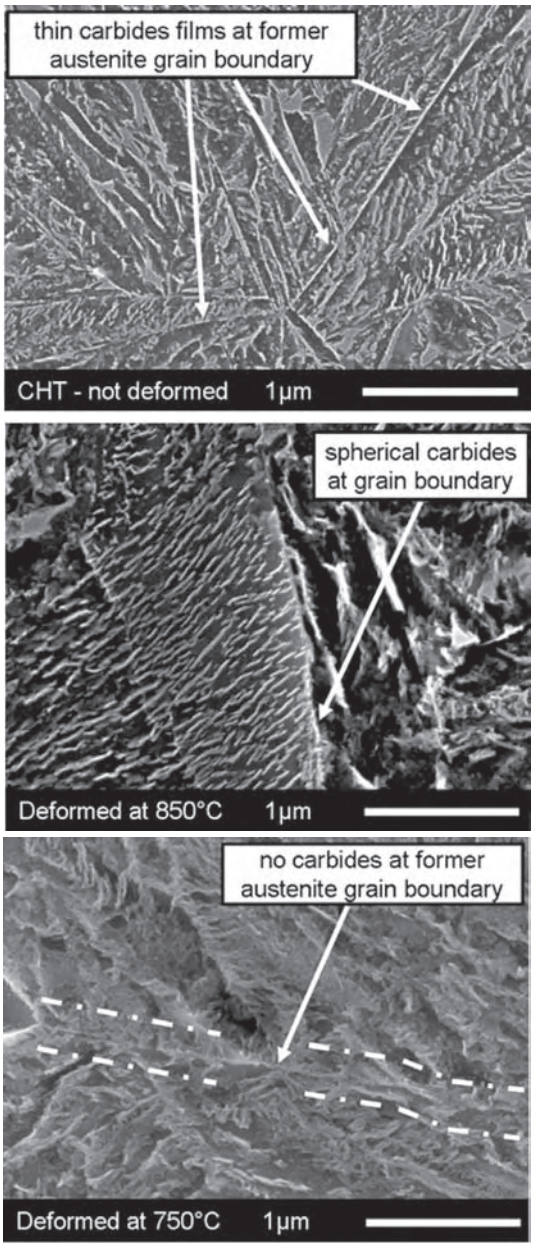

Fig. 4: *Scanning electron micrographs of 55SiCr6 samples with 0.54Cu tempered at 350°C; top: conventional heat treatment; centre and bottom: thermomechanical treatment.*

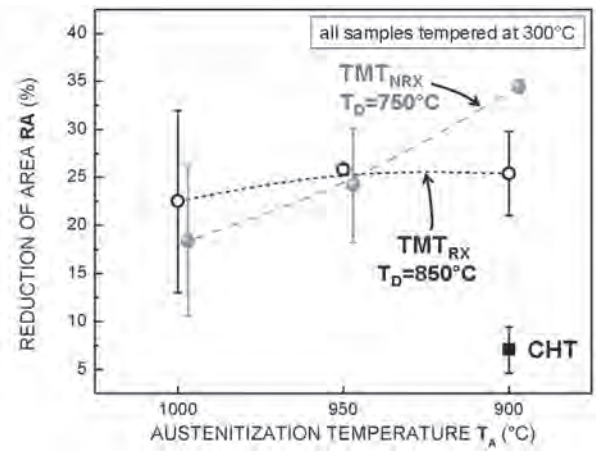

Fig. 5: *Influence of austenitization temperature on ductility for CHT and TMT (55SiCr6 with 0.021 mass % phosphorus).*

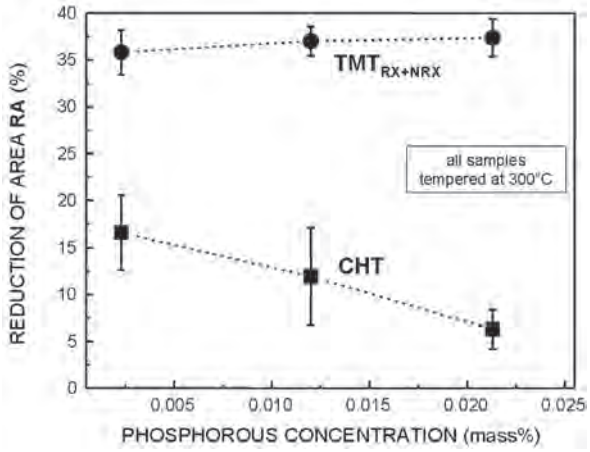

Fig. 6: *Reduction of area of CHT- and two-step TMT samples after tempering at 300°C (55SiCr6 with different P-content).*

The results show that not only deformation at low temperatures but even at deformation temperatures above the recrystallisation temperature lead to remarkable improvements of the properties. A higher deformation temperature reduces the difficulties of applying thermomechanical treatment in technical production processes. Addition of microalloying elements like vanadium can further be used to refine the austenite grain size during austenitization or enhance the possibilities of microstructure control by a thermomechanical treatment.

Acknowledgements. Results presented here are from the research project AiF 13409N. Funding was provided by the German Federal Ministry of Economics and Labour (BMWA) via the German Federation of Industrial Cooperative Research Associations „Otto von Guericke“ (AiF) and the Steel Forming Research Society (FSV). The long version of the final report can be ordered from the FSV, Goldene Pforte 1, D-58093 Hagen.

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Thermodynamic and Kinetic Aspects of the Selective Surface Oxidation of Binary, Ternary and Quaternary Model Alloys

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Department of Interface Chemistry and Surface Engineering

Oxidation of alloying elements (Si, Mn, Cr, Al, etc.) used in new high strength steel grades generally makes steel surfaces unsuitable for subsequent galvanising, as the wettability of these oxides with zinc is generally known to be very poor [1-4]. Hence it is important to investigate the surface characteristics (i.e. change in surface chemistry) of model alloys during industrial annealing. The aim of the present investigation is to understand the influence of annealing conditions and the effect of alloying elements on the surface chemistry and selective oxidation of binary (Fe-2Si, Fe-2Mn and Fe-0.8Cr), ternary (Fe-2Mn-2Si, Fe-2Mn-0.8Cr, and Fe-2Si-0.8Cr) and quaternary (Fe-2Mn-2Si-0.8Cr) model alloy systems. Earlier investigations on oxidation behaviour of Fe-Si and Fe-Mn alloys [5-9] show that during annealing only SiO_2 and MnO are stable on the surface. However, the formation of mixed or complex oxides is possible in the ternary and quaternary alloys. Based on Wagner's theory, transition from external to internal oxidation is achievable by choosing an appropriate dew point in the annealing atmosphere [10]. Increasing the dew point increases the oxygen partial pressure, so the permeability of oxygen into the alloy increases and internal oxidation is supposed to occur.

Short term annealing experiments were carried out using a horizontal infrared heating furnace (Quad Ellipse Chamber, Model 5528-10, Radiant Energy Research). The annealing atmosphere used was a 95%N_2 and 5% H_2 gas mixture, the flow rate was 5 l/min. The dew points used during these investigations were –80 ^{0}C and –40 ^{0}C. The samples were first characterized by X-ray photoelectron spectroscopy (XPS) followed by scanning electron microscopy (SEM). The bonding state of the elements i.e. surface chemistry was studied using a Physical Electronics Quantum 2000 scanning ESCA microprobe. In order to obtain an oxide scale thickness, the XPS sputter depth profiles were measured and sputtering was done with 2 KeV Ar^+ ions in steps of 2 to 3 nm. The sputter rate was calibrated by using an oxidized silicon wafer of known oxide thickness In order to quantify the elemental depth profiles; CASA XPS software (with appropriate sensitivity factor) was used. The elemental spectra were fitted with Gaussian-Lorentzian lines and Shirley background type was used.

At this dew point –80 ^{0}C, the calculated partial pressure of oxygen is ~1.43 ×10^{-28} bar and high enough to oxidise Si and Mn in the binary alloys and at the very border for oxidation of Cr (~6.9 ×10^{-28} bar) [11]. The major contributions of the Si 2p spectrum at binding energy of 104.6 eV correspond to SiO_2 on the surface [9]. The weak component at 102.3 eV indicates the presence of fayalite (Fe_2SiO_4). The fayalite (Fe_2SiO_4) formation is possible where the formed SiO_2 reacts with FeO (2FeO + SiO_2 = Fe_2SiO_4) formed during cooling. Only one component is present at 640.9 eV in the Mn2p spectrum which corresponds to MnO [13]. On the surface of the Fe-0.8Cr alloy, the Cr2p spectrum is fitted with one component at 576.5 eV assigned to Cr_2O_3 [13]. After annealing at dew point –40 ^{0}C, the Si2p spectrum) fitted well with single component at 104.3 eV i.e. to SiO_2. Two components are necessary to obtain a reasonable fit for the Mn2p spectrum. The lowest binding energy component at 640.8 eV (23.42%) is assigned to MnO whereas the rest of the peak envelope is Mn_3O_4 with a binding energy of 641.9 eV (76.58%) [9]. The Cr2p spectrum is fitted with one component at binding energy of 577.2 eV which is attributed to Cr_2O_3 [15].

The Si 2p spectrum of the oxidised ternary Fe-2Mn-2Si alloy annealed at DP – 80°C can be fitted with two components. The higher intensity component (contribution of 60.47%) is at 104.2 eV and attributed to SiO_2 [9]. The additional component at 102.1 eV (contribution of 39.53%) confirms the presence of Mn-Si mixed oxides ($MnSiO_3$/Mn_2SiO_4) [2,14]. The high intensity component of the Mn2p spectrum at 642 eV of this alloy is supporting the formation of $MnSiO_3$/Mn_2SiO_4 [2,12]. The weak component (at 640.9 eV) of contribution 6.18% in Mn2p spectrum reveals the presence of MnO. On the surface of the oxidised Fe-2Mn-0.8Cr alloy, the fitted component at 640.9 eV in the Mn2p spectrum belongs to MnO. The Cr2p peak position at ~576 eV corresponds to Cr_2O_3 [13,15]. Surface analysis of the oxidised Fe-2Si-0.8Cr alloy shows the fitted peak position for silicon at 103.2 eV attributed to SiO_2 [13]. The Cr 2p spectrum of this alloy is fitted with two components; a higher intensity component (of contribution 86.24%) at 577.1 eV refers to Cr_2O_3 and the second component at 574 eV to metallic Cr. On the surface of the oxidised Fe-Mn-Si annealed at DP –40°C only one component

is present at 102.7 eV in the Si2p spectrum which is attributed to Mn-Si mixed oxides. The Mn2p spectrum is fitted with two components at 642.8 eV and 641.7 eV with respective contributions of 72.85 and 27.15%. Despite of their slight shift in the binding energies in both (Si2p and Mn2p) spectra, they can be assigned to $MnSiO_3/Mn_2SiO_4$ and MnO/Mn_3O_4, respectively. Analysing the surface of the Fe-2Mn-0.8Cr alloy, the Mn2p spectrum is fitted with two components. An high intensity component of contribution 76.4% at 641.9 eV belongs to Mn_3O_4, whereas the second component (23.6%) at 640.6 eV belongs to the Mn-Cr mixed oxides ($MnCr_2O_4$) [13]. The Cr2p peak position is also fitted with two components of positions at 577.2 eV and 576.2 eV, assigned to $MnCr_2O_4$ and Cr_2O_3 , respectively. The fitted component position for silicon on the surface of the Fe-2Si-0.8Cr alloy is at 103.9 eV and attributed to SiO_2However, in-depth observation on this alloy gives the evidence for the presence of Cr_2O_3 along with metallic Cr in the near-surface region.

The peak position of the Si2p spectra of both dew points clearly indicates the presence Mn-Si mixed oxides, i.e. $MnSiO_3/Mn_2SiO_4$. on the surface of the annealed quaternary alloy. For both dew points the Mn2p peak in the spectrum can be fitted with two components. At low dew point, both components are located at 642 eV ($MnSiO_3/Mn_2SiO_4$) and 640.9 eV (MnO) respectively. Their intensities lead to estimates of the contribution of two components as follows: 91.9% and 8.1%. At high dew point, (as mentioned in the binary and ternary alloy sections) MnO/Mn_3O_4 is observed along with the Mn-Si mixed oxides. In this case, contributions of the fitted components are as follows: 80.01% and 19.99%, respectively. The Cr2p peak position of the quaternary alloy annealed at low dew point belongs to metallic Cr. However, it can be fitted with shoulder component at 576.7 eV (55.08%) which corresponds to Cr_2O_3. The reason is that, at lower dew point –80 ^{0}C, the partial pressure of oxygen is not high enough to oxidize Cr completely. At higher dew point –40 ^{0}C, well pronounced Cr2p spectra clearly confirm the presence of Cr_2O_3. The XPS depth profiles of quaternary alloy annealed at both dew points are shown in the Figs. 1a and 1b. At low dew point, the oxide scale thickness is about 10 nm. At higher dew point, the oxide scale thickness appears to be more than 32 nm. In this case, Si and Mn indicate the presence of Mn-Si mixed oxides throughout the depth profile and the existence of Cr-oxides is also confirmed in the entire profile. Interestingly, in-depth quantification shows that the amount of Cr_2O_3 increases with increasing depth at higher dew point, obviously due to internal oxidation of Cr. On the other hand, Si and Mn oxides (as Mn-Silicate) are observed maximum on the surface and their concentration decreases in depth.

Binary alloys Fe-Cr and Fe-Si form monophase oxides Cr_2O_3 and SiO_2. In the Fe-Mn system, an increase of the dew point leads to the formation of Mn_3O_4 along with MnO, which was found as the only component at lower DP. The quantification of the oxide forming elements on the surface of the binary alloys shows that at low DP the enrichment of Si is much higher (due to its higher affinity to oxygen) compared to the concentrations of Mn and Cr. At higher DP, the concentration of Mn and Cr increases, due to the higher oxygen potential.

It is very clear when Mn is alloyed with Si, $MnSiO_3$. as well as Mn_2SiO_4 is formed. The formation of mixed oxides is favourable for two reasons: First, the diffusion coefficients for Si and Mn in ferrite [D(Si) = 2.29×10^{-11} cm^2/sec and D(Mn) = 1.41×10^{-11} cm^2/sec] are nearly the same at ~820 ^{0}C which causes their co-segregation and subsequent oxidation according to the following reactions (1,2)

$$MnO + SiO_2 = MnSiO_3 \quad (1)$$

and

$$2MnO + SiO_2 = Mn_2SiO_4 \quad (2)$$

Second, the values of standard free energy ΔG^0 and free energy $\Delta G_{T,P}$ of the formation of $MnSiO_3$ and Mn_2SiO_4 a very negative, as calculated by using the formula given below [18]:

$$\Delta G_{T,P} = \Delta G^0 + RT \ln [p(H_2)/p(H_2O)]$$

where $\Delta G^0 = -303.3 - 21.3\times10^{-3}T$ (for $MnSiO_3$) and

$\Delta G^0 = -412.8 - 39.0\times10^{-3}T$ (for Mn_2SiO_4).

The free energy of $MnSiO_3$ formation at both dew pints -80 ^{0}C and –40 ^{0}C are –1262.98 kJ/mol and –1312.86 kJ/mol respectively. For Mn_2SiO_4, these values are more negative and they are listed as follows, –1802.33 kJ/mol (for DP –80 ^{0}C) and –1852.21 kJ/mol (for DP –40 ^{0}C) respectively.

In the case of Fe-Si-Cr ternary alloys, the binary oxides SiO_2 and Cr_2O_3 are present at both dew points, since no mixed oxides of Si and Cr are formed. It is interesting to note that in contrast to the binary alloy Fe-Cr, also metallic Cr was detected at low DP. This incomplete oxidation of Cr may be attributed to kinetic factors in the sense that surface oxygen is consumed basically by oxidation of silicon. The smaller amount of silicon is a result of a share of available oxygen atoms between Cr and Si, whereas not all the chromium can be oxidised. On the surface of the Fe-Mn-Cr alloy, there is no significant enrichment of Mn and Cr at low DP. At DP –40°C, Mn-Cr mixed oxides are formed according to:

$$MnO + Cr_2O_3 = MnCr_2O_4 \quad (3)$$

According to the phase stability diagram in FactSage™ data base, the Mn-Cr mixed oxides (i.e. $MnCr_2O_4$) are more stable at higher dew point, because the oxidation of manganese is more pronounced. Consequently, at DP –80 ^{0}C, only binary oxides MnO and Cr_2O_3 are formed. There is also a slight tendency for internal oxidation of chromium in Fe-Cr and Fe-Mn-Cr alloy since the chromium concentration increases slightly with increasing depth. This can be explained on the basis of permeability calculations for oxygen and Cr by using the equations given in extended Wagner's model proposed by Huin et al [17]. Increasing the dew point, i.e. increase of surface oxygen content in the annealing atmosphere leads to the higher inward oxygen permeability. At increased dew point -40 ^{0}C, Cr is on the very border for internal oxidation, i.e. $D_OO_S >> D_{Cr}Cr_B$ where D_O and D_{Cr} are the diffusion coefficients of oxygen and Cr. The surface oxygen concentration and elemental Cr bulk concentration are represented as O_S and Cr_B respectively. The calculated inward oxygen permeability D_OO_S at high DP is 3.98×10^{-13} cm^2/s whereas the outward Cr permeability $D_{Cr}Cr_B$ is 5.16×10^{-12} cm^2/s, which is on the very border for chromium external/internal oxidation. When Si is alloyed with Cr, the distribution of Cr decreases almost linearly from the surface to the oxidation front, i.e. the in-depth Cr-oxidation is suppressed by decreasing the surface oxygen potential down to that of silicon which, in turn, leads to more external oxidation of Cr.

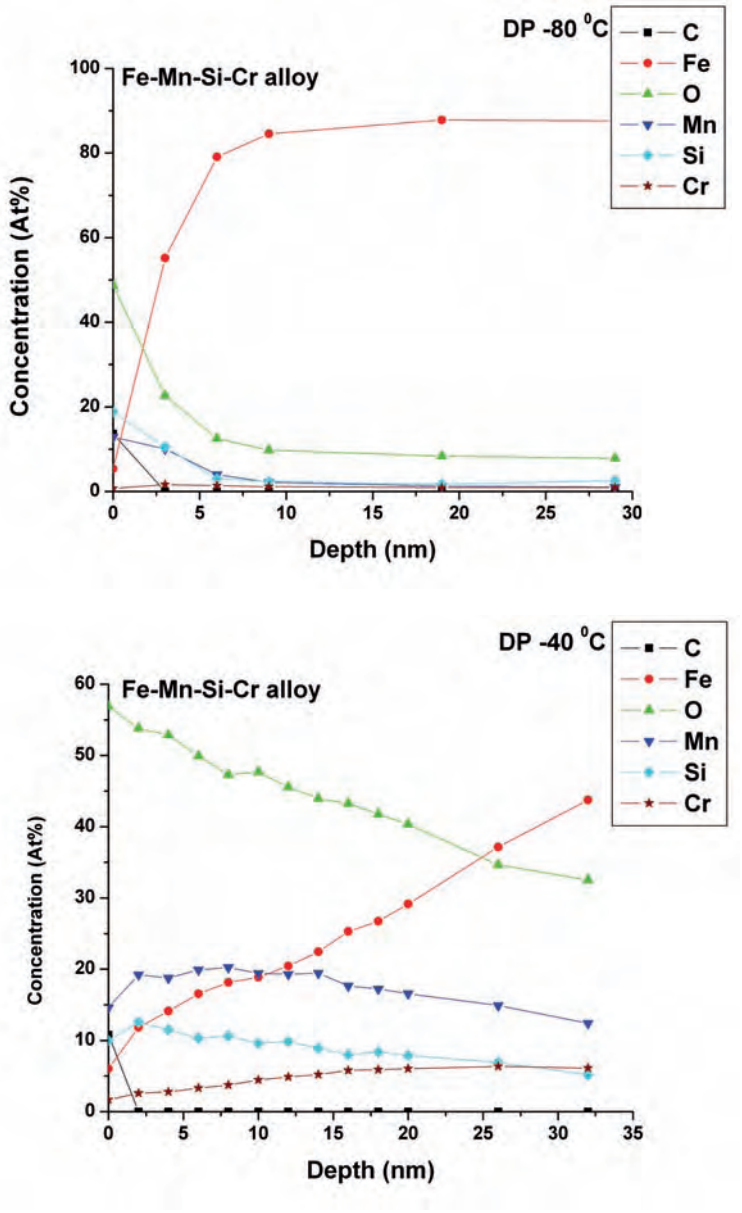

Fig. 1: *The XPS depth profiles (a: DP -80 ^{0}C, b: DP -40 ^{0}C) of the annealed quaternary model alloy.*

Upon oxidation of the Fe-Mn-Si-Cr alloy, mainly Mn-silicates are formed as ternary oxides showing that the affinity between Si and Mn is obviously higher than between Mn and Cr. By closely observing the Cr peak positions, it clearly shows the formation of only Cr_2O_3 in the entire profile, leading to the conclusion that there is no interaction of Cr with Mn in the quaternary system. When Si and Mn alloyed together with Cr in the quaternary alloy, the Cr concentration is increasing with increasing depth, showing a clear trend for its internal oxidation. Obviously, the formation of Mn-Si mixed oxides prevails thus hindering the interaction of Mn with Cr and , therefore, suppressing its segregation to the surface and consequently internal oxidation of Cr occurs .

In conclusion, on the surface of the binary alloys only binary oxides are formed i.e. SiO_2 (Fe-Si) and Cr_2O_3 (Fe-Cr) independent of the dew point. In the case of Fe-Mn, MnO is formed at low DP and additional Mn_3O_4 at higher DP. By presence of Si and Mn in the system, the formation of $MnSiO_3$/Mn_2SiO_4 takes place on the surface at both dew points.

When Mn and Cr are present in the alloy, they show also chemical interaction by forming $MnCr_2O_4$ at DP –40 ^{0}C apart from their own oxides Mn_3O_4 and Cr_2O_3. Si and Cr are forming their binary oxides i.e. SiO_2 and Cr_2O_3 at every DP without any interaction between them.

In the quaternary system (Mn with Si and Cr), Mn interacts only with Si by forming manganese silicates, although Mn showed its interaction with Cr in the ternary system. Obviously, Mn has higher affinity to Si than to Cr. Annealing at higher dew

point -40 ^{0}C increases the oxygen partial pressure in the annealing atmosphere and favours the trend for internal oxidation of Cr with increasing in-depth distribution of Cr-oxides.

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Theory-Guided Design of Metallic Alloys

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Computational materials design is a rapidly evolving multidisciplinary field of rapidly growing importance. The primary goal is a predictive understanding of materials properties what requires a clear picture of the role played by atomistic processes in determining the materials behavior. State-of-the-art approaches employ fundamental quantum mechanics approaches describing accurately the behavior of electrons and thus of chemical bonds in a solid. Its successful performance is strongly enhanced when new computational algorithms and exponentially increasing computer power are efficiently combined with cross-checking verification by experimental measurements. Theoretical predictions may serve here as a guide when new materials with desired physical and chemical characteristics are to be designed and built. The potential and strength of this ab initio approach will be demonstrated on two examples: (i) an investigation and interpretation of the volume-composition anomaly detected in Fe-Al alloys and (ii) identifying strategies to design biocompatible Ti-binaries for medical application. The first phenomenon is closely related to the development of new light-weight Fe-Al materials with optimized properties. The second topic is aimed at an improvement of hip transplants and addresses the lack of suitable materials which are biocompatible in terms of non-toxicity and mechanical properties matched to the bone.

Volume anomaly in Fe-Al alloys. Iron aluminides represent a promising class of intermetallics with great potential for substituting stainless steels for applications at elevated and high temperatures. Noteworthy in this respect is their excellent chemical resistance with respect to corrosion and sulfidation processes, low cost of the constituents, high strength, and a lower density compared to that of many other iron-based materials [1]. Numerous attempts to reduce the density of the materials have been hampered by the fact that the dependence between the alloy composition and volume is rather complex: several experimental studies observed an anomalous, strongly non-linear behavior in a large part of the concentration range [2-4] (see black and red symbols in Fig. 1). The study of the volume-alloy

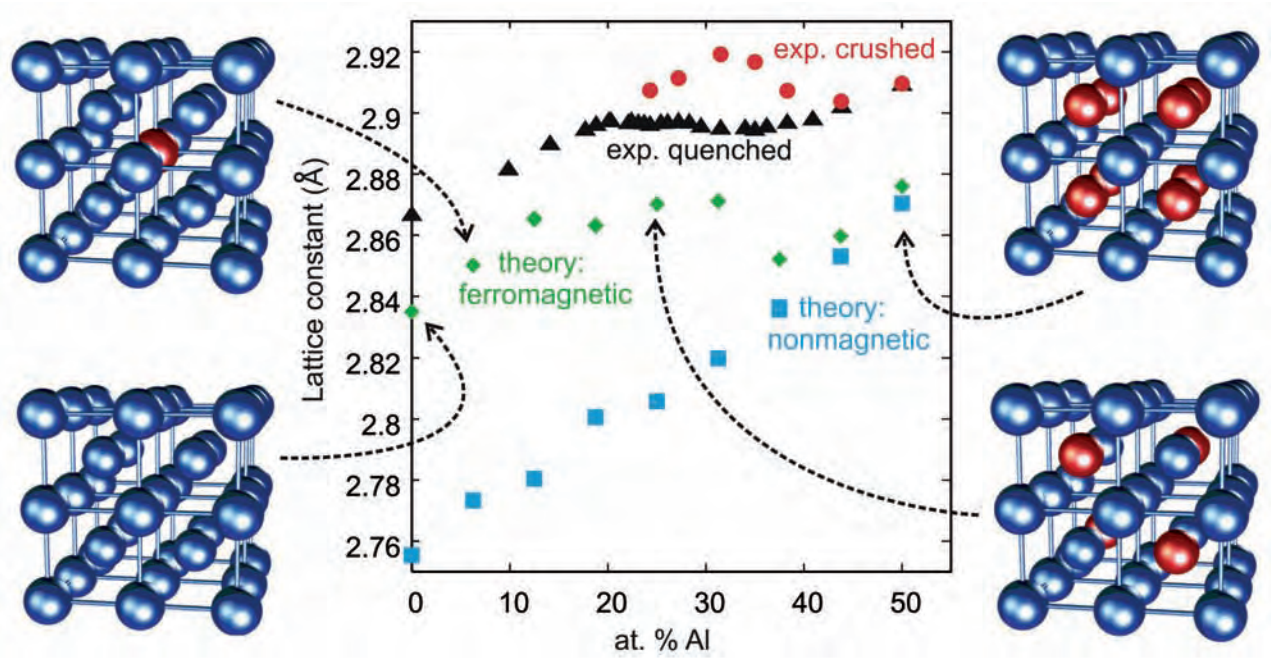

Fig.1: *Compositional lattice-constant dependence of the Fe-Al alloys. Both experimental measurements [2] (black and red symbols) and theoretical prediction for the ferromagnetic (green) and nonmagnetic (blue) states are displayed. Examples of crystal structures are shown for pure iron and 6.25 at. % Al alloy (bottom and upper left) as well as $D0_3$ structure of Fe_3Al and B2 phase of FeAl (bottom and upper right).*

dependence has been further complicated by the fact that the functional behavior of the dependence turned out to be not unique but to depend on the processing history (thermal and mechanical treatment) of the sample studied. Measured lattice constants consequently cover quite a broad range of values with the lower limit represented by the quenched samples and the upper by the crushed ones [2].

In order to identify the origin of the anomaly observed for the crushed samples we have performed theoretical calculations of Fe-Al alloys with various compositions and local order employing density functional theory [5,6]. In the theoretical study the focus has been on the Fe-rich part of the Fe-Al phase diagram where all the structures are derived from the cubic body centered (bcc) structure of pure iron. The research had to deal with the structural complexity of the alloys that are (i) substitutionally disordered up to 18 at. % of Al, and (ii) changing the structure with increasing Al content through $D0_3$ found in Fe_3Al to B2 in case of FeAl. In the calculations, the binary alloys have been described by periodically repeated supercells consisting of 2x2x2 elementary cubic unit cells with a total of 16 atoms. A large variety of alloy compositions and atomic configurations (23 in total) has been studied this way by systematically replacing Fe atoms by Al atoms. For each concentration the lattice parameter has been estimated as the average over different atomic configurations weighted with respect to the energy of each configuration. The lattice parameters calculated in this way are depicted as green diamonds in Fig. 1.

The FM states clearly show a strong anomaly that reproduces the main characteristics of the experimentally measured data including the drop of the lattice constants between 30 and 40 at. % of Al. A closer analysis showed that the composition region where the anomaly occurs shows a rapid collapse of the magnetic moments of the Fe. This finding is consistent with experimental measurements of a rapidly decaying magnetic moment in this range of compositions [2].

A great advantage of the theoretical simulation is that the origin of mechanisms such as the volume anomaly here can be studied in a unique way. For example, to study and quantify the effect magnetism has on this feature we can perform a fully analog study but with the magnetic moment fully switched off. We therefore have repeated the calculations for alloys containing solely nonmagnetic (NM) iron atoms (blue squares in Fig. 1). In contrast to the FM states, the lattice constants of the NM states show an almost linear dependence without any anomaly. We can therefore conclude that the volume anomaly in Fe-Al alloys is driven by a magneto-volume instability and not by an order-disorder transition.

Bone-matched Ti-alloys. The second example of our approach describes a theory-guided search for novel materials for human implants. The highly corrosive environment of human body combined with the poor tolerance to even minute concentrations of most metallic dissolution products eliminates most metals from use as implant materials. Moreover, the non-toxic materials must obey another vital condition, mechanical compatibility, which means here that the bone and the metal alloy should have elastic properties which are closely matched. The mechanical compatibility may be expressed as the match in the Young modulus between bone (with the Young modulus value between 20 and 30 GPa) and implant material. If this compatibility is given, the bone regeneration and repair are promoted by the mechanical load on the bone. However, the metals presently used for bone implants are much stiffer than the bone and the implant carries a disproportionate amount of the biological loads. The surrounding bone is then “stress-shielded” and experiences abnormally low levels of the load. This non-compatibility often causes functional failure via re-sorption of the bone and loosening of the implant [7].

The class of metastable Ti-alloys with cubic structure seems to have very promising mechanical properties. Stimulated by a current effort to design new materials with improved biocompatibility, we have studied Ti-alloys containing exclusively non-toxic element (Ti and Nb) and selected those with the best mechanical compatibility with human bone. Due to the fact that the cubic phase is the high-temperature phase of Ti-Nb alloys, materials are usually obtained via quenching from the temperature region above the transition temperature into a low-temperature, hexagonal close-packed (hcp) phase. The metastable character of the alloys is reflected in the fact that only alloys with Nb-content higher than 23 at. % Nb are thermodynamically stable at ambient temperatures [8].

Current experimental studies of the mechanical properties are facing problems related to the polycrystalline and multi-phase character of the samples. A main advantage of the theoretical approach is the possibility to study a single crystal or process individually, i.e., without having to consider the complexity of the whole system. This approach allows to efficiently analyze the properties of a selected phase or mechanism and to determine the contribution of a single phase to the whole system.

For the investigation of the Ti-Nb binaries were we employed the same supercell approach as in case of the Fe-Al alloys above. As a measure for the mechanical compatibility between implant and alloy the Young modulus has been identified as the relevant quantity. The Young modulus has been

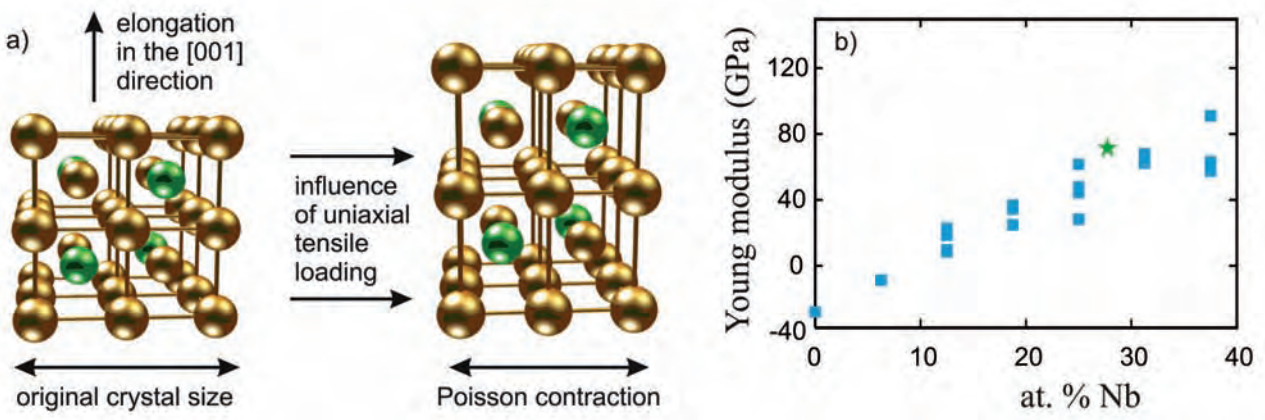

Fig. 2: *Schematic representation of theoretically simulating tensile loading in the [001] direction for the example of a crystal in $D0_3$ structure (a). The calculated values of the Young modulus of the Ti-Nb alloys are shown in (b). At each alloy composition the Young moduli of all supercells with that particular composition but different local atomic order are given. The green star in (b) represents the data from the experiments and measurements performed in the Department of Microstructure Physics and Metal Forming.*

calculated by performing a simulation of a uniaxial tensile test in the [001] direction (see Fig. 2a). A detailed description of the methodology used for the calculations of the Young modulus is given in Ref. [9]. The results are displayed in Fig 2b. As can be seen, the Young modulus increases almost linearly with the alloy composition. The values for thermodynamically stable alloys with ~ 25 at.% Nb are very close to the range typical for the human bones (20-30 GPa). It is interesting to note that for the lowest alloy compositions (i.e., close to the limit of pure Ti) the Young modulus becomes negative. A negative Young modulus implies that for low Nb concentrations these alloys are mechanically unstable against tetragonal deformations. This conclusion is in agreement with previous studies on the elastic stability of bcc Ti (see e.g. [10]).

An integral part of the collaborative theoretical and experimental activity was the verification of the theoretically predicted metallurgical trends. Therefore, in the Microstructure Physics and Metal Forming Department Ti-Nb alloys have been cast, processed and measured. Specifically, a high purity Ti-alloy with 30 at. % Nb was prepared in an electric arc furnace which provided an intense stirring effect. In order to obtain excellent cast samples of maximum chemical and structural homogeneity the specimen was remelted several times. The elastic properties were then investigated by using an ultrasonic resonance frequency method measuring the elastic modulus by analyzing the natural period of the transient vibration which results from a mechanical disturbance of the object tested (Grindo-Sonic).

The measurement was performed on a *polycrystalline* sample. Thus, the Young modulus is now an averaged quantity. The averaging goes over many grains with varying crystallographic orientation. The fact that the values of the Young modulus in other directions are expected to be higher than in the [001] direction, is consistent with the fact that the (averaged) measured value is higher than the (anisotropic) theoretical value (Fig. 2b). Nevertheless, even though the preliminary theoretical studies do not cover the full complexity of the system, important trends can be derived: The mechanical instability along the [001] direction identified by theory shows an interesting route to design Ti-based alloys with low values of the Young modulus.

The two examples discussed here show that ab initio based theory-guided design in close connection with experiment can be an efficient tool in the hands of modern materials scientists.

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Microstructure-Related Materials Properties

Introduction

The interdisciplinary field of “Microstructure-Related Materials Properties“ represents an area of strong overlap among the departments.

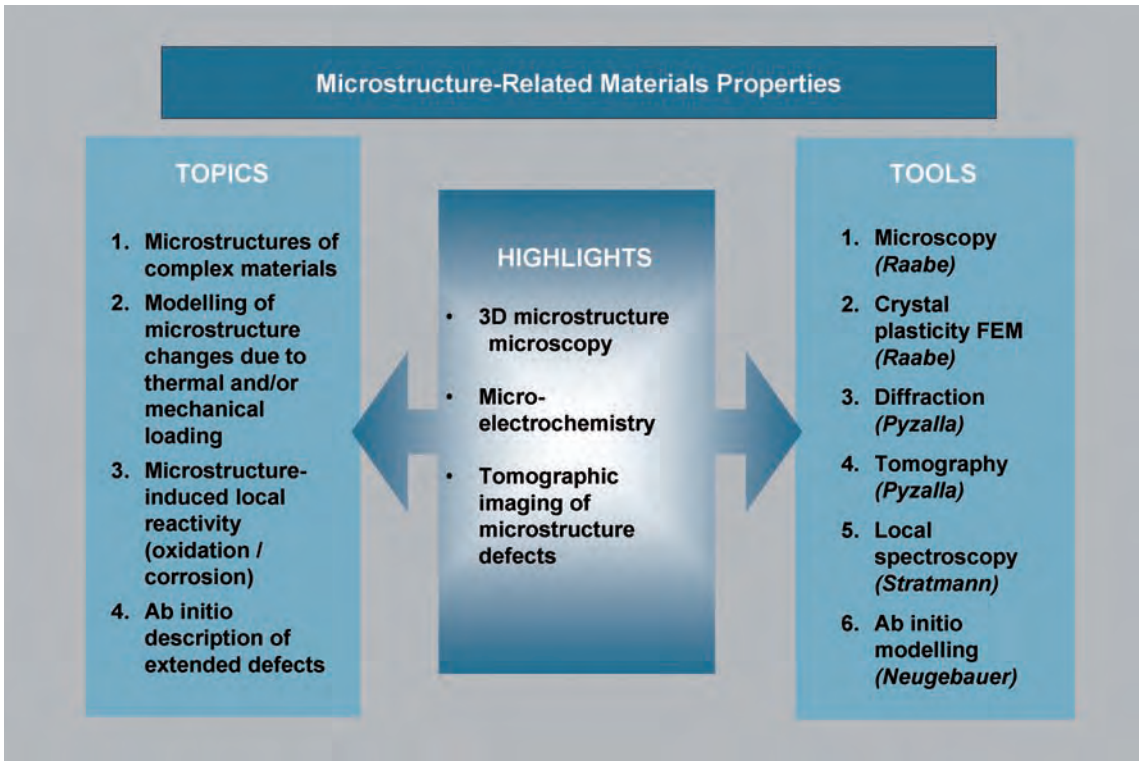
Modern materials science is based on the fundamental experience that the properties of materials are not unalterably determined by their average chemical composition but they are to a large extent influenced by their microstructure. This applies particularly for their mechanical properties. Thus, modern engineering materials development strategies are often closely associated with advanced fundamental microstructure research.

While the evolutionary direction of microstructure is prescribed by thermodynamics, its actual evolution path is selected by kinetics. It is this strong influence of thermodynamic non-equilibrium mechanisms that entails the large variety and complexity of microstructures typically encountered in steels and related engineering materials. It is an essential observation that it is not those microstructures that are close to equilibrium, but often those that are in a highly non-equilibrium state that provide particularly advantageous material property profiles.

During the last decade the field of microstructure-oriented steel research has worldwide undergone a tremendous gain in importance, for science, economy, and society. This observation can be explained in the light of three main developments.

The first one has an economical background, namely, the enormous increase in the industrial usage of steel and related materials owing to the large request particularly of the automotive and construction industry and the resulting increase in steel price.

The second one is the strong pull effect which is exerted by new exciting developments which we currently see in the main application fields for steels. In this area particularly the accelerating introduction of novel high strength steels and advanced manufacturing methods in the automotive industry must be named. The third factor is that both fundamental and applied steel research have entailed a number of essential breakthroughs particularly in the domain of high strength steels. These new materials exploit the hardening and ductility effects associated with complex deformation-induced transformations



and multiple twin formation exceeding the properties of steels which are currently in use in part by a factor of two or more. Similar developments have taken place by producing constructional steels with ultra fine grains down to the nanometer regime. Many of these new steels can be characterized as materials with an ultra-high density of interfaces.

The benefits resulting from these recent positive developments in the field of steel research are at hand: Stronger steels allow for novel advanced light-weight engineering solutions entailing huge energy savings and safer constructions. Since these new materials often occupy essential bottleneck functions in our modern high-technology society, they allow for the design of new products which could not be created before. Modern steels with complicated microstructures also create a pull effect in the field of fundamental research to better understand the basics of these materials through the aid of novel advanced characterization approaches such as synchrotron tomography, high resolution 3D orientation microscopy or new theoretical approaches such as the employment of quantum mechanics for the ab-initio design of new alloys.

It is obvious that the current dynamic situation in that field creates huge possibilities and challenges in the field of microstructure research.

Therefore, the following collection of project reports is devoted to this exciting field addressing such diverse topics as high-strength wire production, directionally solidified eutectics, 3D-orientation electron microscopy, microstructure and properties of biological composites, advanced synchrotron X-ray diffraction and tomography methods, and fundamental multiscale modeling studies on interfaces in metals.

It is hoped that these short reports give an impression of the strong links between complex microstructures, improved properties, and applications in the field of advanced engineering materials which are in the focus of this institute.

Continuous Production of High Strength Wires and Softmagnetic Thin Wires and Fibres

S. Zeller, J. Gnauk, G. Frommeyer

Department of Materials Technology

The MPIE possesses great experience in the development of near net shape casting technologies, starting with the twin-roll strip-casting facility and the direct casting of ribbons and foils (planar flow casting, meltspinning) up to the casting of wires (shape flow casting, SFC [1,2]) and fibres (In-Rotating-Liquid-Spinning, INROLISP [3-5]). The processes are analysed and optimised with respect to the process technique and the material science.

The produced fibres provide a metastable, fine grained, partly crystalline or even amorphous structure, exhibiting enhanced strength and elastic properties in contrast to conventional solidified material. Of high interest are the special soft magnetic properties of rapidly solidified ferromagnetic alloys.

Softmagnetic amorphous and nanocrystalline CoFeSiB and FeSiB microwires are used to develop high sensitive magnetic field sensors, working at room temperature. Therefore, a quasilinearly depending alternating induction voltage U_p is generated in a pickup coil, located coaxially around the microwire sensor core, while the external magnetic field is detected (Procopiu effect) [6].

Continuous casting of wires. In the SFC-process – direct casting on a rotating profiled substrate surface – pure metals or alloys are molten and superheated under inert gas atmosphere in high-temperature resistant ceramic or quartz crucibles. After applying argon excess pressure, the melt exits the nozzle as a free jet and strikes the rotating surface of the substrate at a defined angle α of immersion. The bottom side of the cylindrical jet is stabilised by the semicircular groove of the substrate and the top side by surface tension. Groove diameters ranging from 1.5 to 3 mm have been used to cast wires close to final dimension.

SFC-technology is a combination of the INROLISP (in-rotating-liquid-spinning) and the PFC (planar flow casting) process [5,7]. With its high cooling rate of 10^3K/s the SFC-process belongs to the realm of the rapid solidification technology.

Direct wire casting requires a precise coordination of the process parameters. Fig. 1 shows the basic function of the continuous casting process and a summary of the most important process variables. The filling of the wire cross section, which is fixed by the geometry of the semicircular groove profile, calls for a continuous mass flow d*m*/d*t*, which is defined by the circumferential velocity ω of the melt. The adequate pressure of ejection can be calculated from $dm/dt=\rho\cdot\omega\cdot A$ using Bernoulli's equation for incompressible fluids and the continuity of the process. The calculations were supplemented by experiments in which the ideal mass of a defined piece of wire was calculated from its density and known ideal cross section and compared with the actual mass. By taking measurements of an alloy, it is possible to plot an alloy-specific characteristic curve where the ejection pressure determines the alloy-dependent viscosity η and surface tension σ.

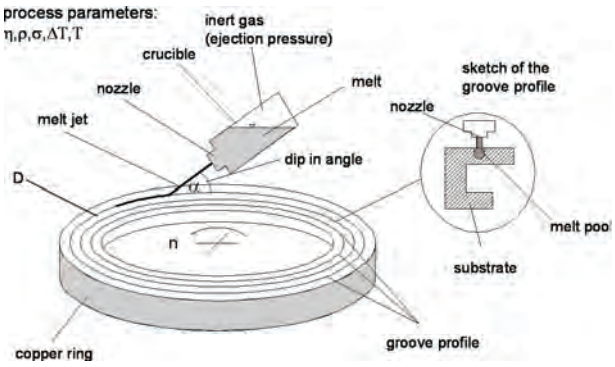


Fig. 1: *Schematic drawing of the SFC-process and the key process parameters, listed up below. η: dynamic viscosity; D: diameter of the groove profile; ρ: density of the melt; σ: surface tension; ΔT: superheat of the melt; T: melting point; α: angle of the melt jet.*

After completing the initial parameter studies on a large variety of metallic alloys with different compositions, melting temperatures, cooling rates, and heat transfer coefficients, the attention was focused on the continuous casting of various austenitic stainless steel wires, ferritic heat-resistant iron-chromium-aluminium alloy and nickel-chromium based material. These alloys are of great importance for industrial applications. Fig. 2 (next page) shows an as-cast stainless steel wire of about *d* = 3 mm in diameter after final dressing and strengthening by cold drawing applying a degree of deformation of η = 15%. The main task was to achieve finer grain sizes by rapid quenching and improved mechanical properties, such as higher strength combined with high production efficiency.

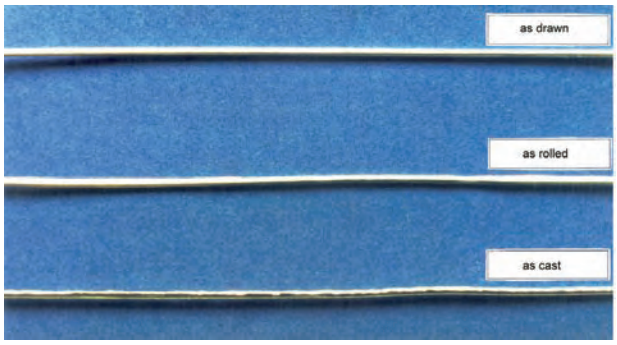


Fig. 2: *As cast stainless steel wire samples after dressing by cold rolling or drawing.*

Casting of fibres and thin wires. In contrast to the SFC process, the diameter of the thin wires produced by INROLISP are not determined by a groove profile but by the nozzle properties. The material is molten and superheated by an induction coil surrounding the crucible and then ejected through a nozzle, applying argon excess pressure. After a free flight of a few millimetres, the melt jet dips into a laminar flowing liquid coolant, where the material rapidly solidifies.

Unlike other comparable facilities, here a horizontal arrangement of the rotating drum is used which provides a much smoother surface of the cooling liquid and an easier process handling (Fig. 3).

In contrast to polyamides or glasses, the metallic melts have a very low dynamic viscosity, which facilitates the ejection of the melt through the nozzle but also destabilises the melt jet. The torque in combination with the surface tension causes a break-up of the jet. Thus, the production of fibres in a stationary process needs an equilibrium between the kinetics of solidification and the fluid mechanic initial disturbances.

Liquids are used as coolant due to the higher heat conductivity in comparison to gases. The liquid coolant has the same velocity as the melt jet, so the effect on the still deformable wire is minimised.

The stability of the melt jet is an important criterion to produce very thin fibres, because the viscosity and surface tension of the melt generate a very short break-up time (≈ 10^{-3} s). The distance between the nozzle and the coolant surface has to be ≤ 10 mm, for a jet velocity of 9 m/s, to solidify the jet as soon as possible and minimise the solidification time. Before the jet enters the coolant, the velocity distribution in the jet is relaxed and a skin zone has grown, which avoids a deformation of the wire entering the coolant surface.

The INROLISP process depends strongly on the break-up length of the melt jet. In contrast to Cu- and Al-base alloys, which have also been casted, Fe- and Co-base alloys possess a much shorter break-up length due to their higher surface tension in the liquid state and other solidification characteristics. Thus, the facility was modified to optimise the orifice geometry and the induction coil to minimise the free flight length to be able to cast continuous wires, which are classified by the University of Düsseldorf regarding their magnetic properties.

Theoretically, the ideal structure for softmagnetic material is an amorphous matrix or a nanocrystalline structure [8]. The structure of the produced wires was examined using optical microscopy, SEM and XRD. In the beginning, the wires had a microcrystalline structure instead of an amorphous matrix as can be seen in Fig. 4. Obviously, the cooling rates were low enough to form a crystalline microstructure in the material. A reason for this low cooling rate is the Leidenfrost-effect, which describes the formation of a steam layer around the hot melt jet and inhibits the direct contact to the coolant. To detain this effect, a polymer solution is used as a cooling medium. The entering jet is now cooled below the glass forming

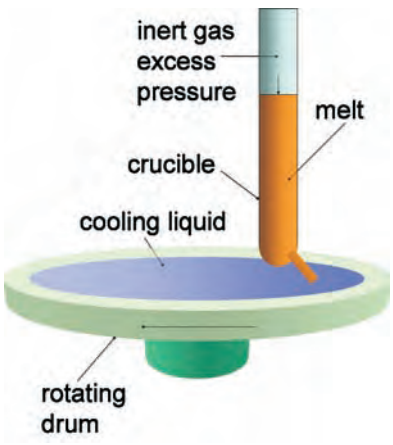


Fig. 3: *The INROLISP-process: The distance from the nozzle to the rotating coolant has to be minimised. The velocities of the coolant and the jet should be nearly matched.*

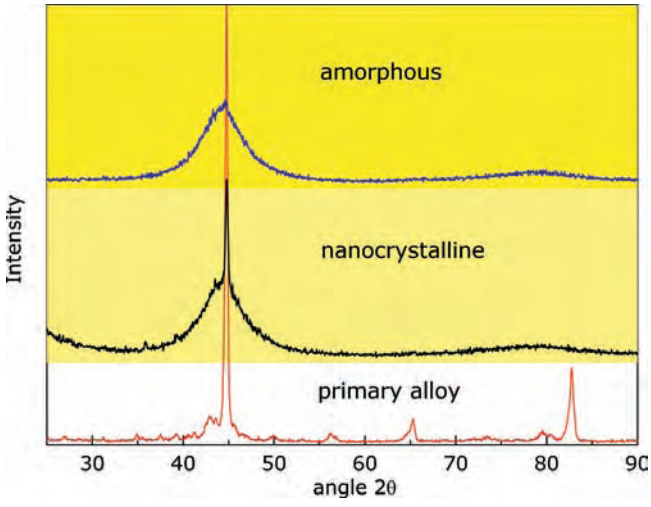


Fig. 4: *X-ray diffraction spectrum of an FeSiB alloy in different cooling levels.*

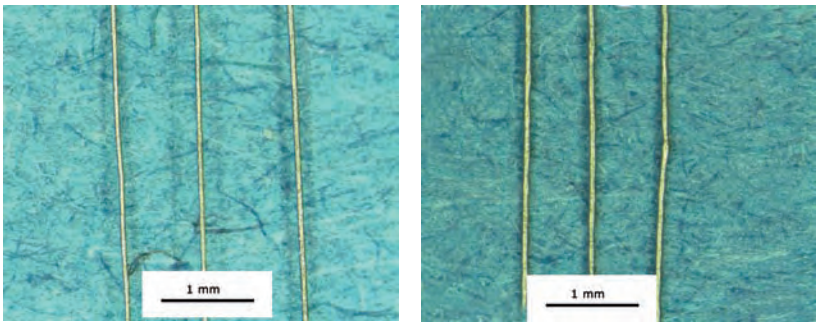


Fig. 5: *Optical stereo micrograph of Co-base wires produced with the INROLISP facility; left: $Co_{66}SiFeNi$, 1283°C casting temperature with 120 µm nozzle; right: $Co_{71}SiBFeNb$, 1267°C casting temperature with 110 µm nozzle.*

temperature T_g and is not disturbed by the coolant. The break-up length of the jet is about 5 mm, the injection angle 60°, the nozzle diameter 100 to 150 µm, the ejection pressure 5 bar, the superheat of the melt 150 K, which results in a jet velocity of 8.3 m/s. The rotation speed should be 20–25% faster than the jet velocity to get plain and smooth wires.

The diameter of the sensor core affects the properties of the Procopiu sensor. Especially the energy consumption and the minimal size of the sensor decrease with smaller fibre diameters.

The appropriate method to influence the geometry of the wire is the variation of the nozzles' orifice, because the nozzles' diameter determines directly the wire shape with a loss of 7-20% of thickness due to the stream relaxation. The used boron-nitride nozzles always are 100 µm in diameter. To get a stronger modification, glass nozzles, ground to a diameter between 50 to 250 µm are used.

The variation of the free flight length, respectively the distance between nozzle tip and coolant surface, determines the uniformity of the wire and allows a prediction on the sensitivity against a varying wire diameter. The wires in Fig. 5 show a periodical disturbance of the wire geometry. A higher ejection velocity reduces these disturbances as preliminary tests with Cu-Al alloys showed.

Most of the wires exhibit a typical casting surface with certain wrinkles due to the contraction of the solidifying material (Fig. 6). Besides the surface and the geometry the structure of a wire is the determining factor.

An amorphous matrix with embedded ferromagnetic nanograins is assumed to be the optimal structure to obtain the softmagnetic effect. The existing results show that already a pure nanocrystalline structure exhibits good, but not optimal softmagnetic properties.

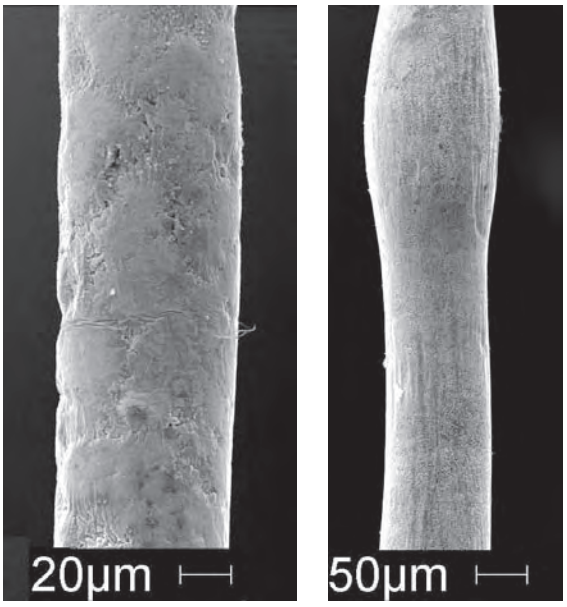


Fig. 6: *SEM-images of the microwires produced by the INROLISP method; left: $Co_{66}SiFeNi$ wire, 110µm; right: $Co_{71}SiBFeNb$ wire, 100µm.*

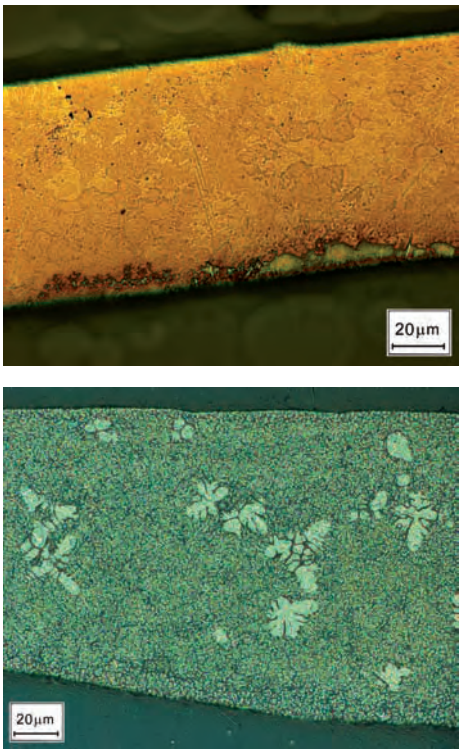


Fig. 7: *Optical micrographs of Fe-base alloys; top: $FeSi_{32}$ wire; bottom: FeSiBNbCu wire.*

Because of the low melting temperature (far below the critical temperature of the glass orifice) and the complete miscibility of all alloying elements, a eutectic $FeSi_{32}$ alloy is used to set up the casting conditions. As can be seen in Fig. 7(a), the grain size is about 15 µm, which is very large for a rapidly solidified material. The comparably long free melt jet length and the Leidenfrost effect are assumed to be the reasons for the too low cooling rates.

Experiments with a quintuple FeSiBNbCu-alloy show again a low cooling rate. Partly it is possible to identify crystalline clusters, exhibiting 20 µm.

It tends to be very difficult to measure single wires with conventional X-ray diffraction, hence at the moment only EBSD scans with a complex sample preparation and extensive measurements can be applied to detect crystalline and amorphous structures in the material. Up to now, a Debye-Scherrer-facility is adapted, to allow a rapid and easy characterisation of the wire.

To get exact data of the solidification, a thermal imaging camera records the process to determine the melt temperature directly before entering the coolant. The solidification conditions can now be determined, calculating the stationary heat balance, with respect to the given boundary conditions.

For a better understanding of the process, a high speed camera observes the free flight length and the penetration of the coolant surface by the melt jet. With these images it is possible to improve the adaptation of the coolant velocity with respect to the jet velocity and to study the fluid dynamic effects like the break-up of the jet experimentally to compare it with numerical solutions.

Continuous casting and rapid solidification of fibres and wires in the diameter range from 50 µm to 3 mm offers many advantages, specifically amorphous state or fine grained semifinished or finished products with improved mechanical properties, high process flexibility and low cost production.

The shape flow casting technology can cut out many forming and heat treatment stages necessary for high quality stainless steel or heat resistant wires of smaller diameters. The achieved cooling rates are high enough for producing the amorphous state and/or finer grain sizes, and less segregations of the alloying and tramp elements in the final wires.

Amorphous softmagnetic wires for high sensitive magnetic field sensor cores in a Procopiu-sensor were synthesised and characterised. The alloy composition is a very important factor, because the softmagnetic properties react very sensitively on a change of the alloy. Hence it is important to investigate and optimise the modification of the Fe- and Co-base alloys – CoFeSiB (e.g. VitroVac6030) or FeSiNbBCu (e.g. FineMet) - and the solidification conditions for the wire and the Procopiu application.

In order to get a better S/N ratio of the sensor, it is planned to reduce the wire diameter to 30–50 µm. A reduction of the diameter results in a decrease in power consumption, which is fundamental for battery or solar energy operated devices.

To build a difference-circuit sensor to compensate interfering fields, a reproducible fabrication of the micro wires is necessary, regarding the alloy composition, the microstructure and the geometry (diameter and alternating disturbances), to guarantee homogenous and uniform magnetic characteristics.

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Electrochemical Processing of Directionally Solidified Eutectics for the Preparation of Various Metallic Nanostructures

A. W. Hassel, B. Bello Rodriguez, S. Milenkovic, A. J. Smith

Department of Interface Chemistry and Surface Engineering

Self-organised metallic nanostructures are pursued for a potential use as arrays in nanotechnology. Nanowires and nanotubes are of special interest as they are 1-dimensional objects that can carry a function on one side and inherently provide a proper connection. Additionally, they provide models for studying the influence of dimensionality and size confinement on electrical transport, optical attributes and other properties. Among the fabrication methods employed, some are based on vapour phase techniques, while others are based on solution techniques. Compared to physical methods such as nanolithography and other patterning techniques, chemical methods have been more versatile and effective in the synthesis of nanowires.

Here, a novel combined method is presented for producing self-organised metallic nanostructures [1,2] which is especially applicable, but not restricted, to metals. It combines directional solidification of eutectic alloys with chemical and/or electrochemical processing. In the first step directional solidification of a eutectic alloy yields self-organised arrays of nanowires of a minor phase embedded in a matrix of the other phase. The process is based on simultaneous crystallization and aligned growth of two phases parallel to the direction of heat extraction (Fig. 1). This method is commonly used to produce high strength materials for application at high temperatures such as turbine blades. Therefore, it may sound contradictory to apply a method that was developed to produce large single crystals to generate nanostructures. Work on solidification, structure and properties of eutectic alloys was recently reviewed by George et al. [3], and was comprehensively treated in a book by Kurz and Sahm [4].

This method has several advantages. First of all, it is one of the few top-down methods that allow the production of large amounts of nanostructures. In addition, both wires and matrix are single crystalline which may favour them for certain applications. Further, the obtained nanostructures exhibit extremely high aspect ratios (>1000), unreachable by most other techniques. Moreover, wire diameter and spacing can be controlled by the processing parameters such as growth rate and temperature gradient (Fig. 2) and show a narrow distribution (Fig. 3) [5]. The method is highly versatile and applicable to a broad range of materials for different applications. Finally, it

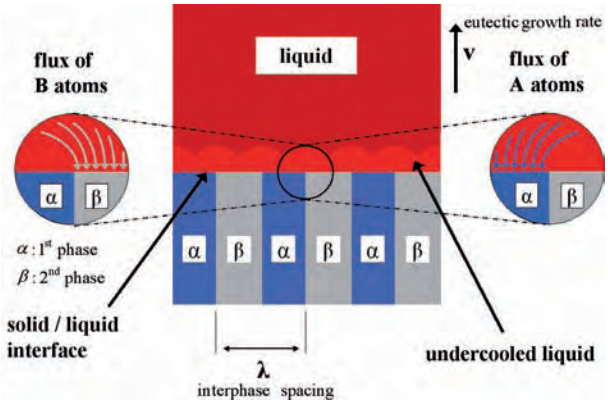

Fig. 1: *Schematic of eutectic coupled growth [1].*

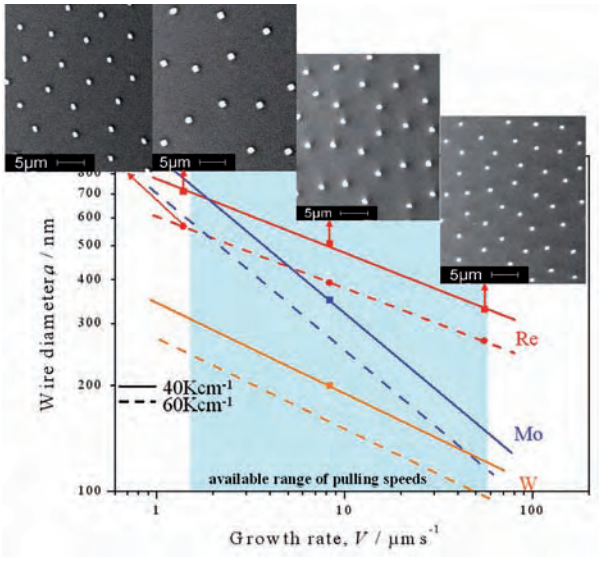

Fig. 2: *Influence of growth parameters on nanostructure features [5].*

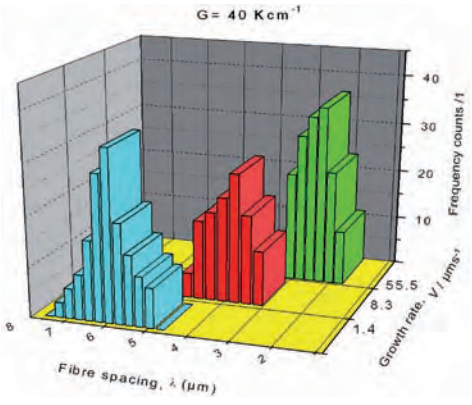

Fig. 3: *Histogram of nanowire spacing for various growth rates [5].*

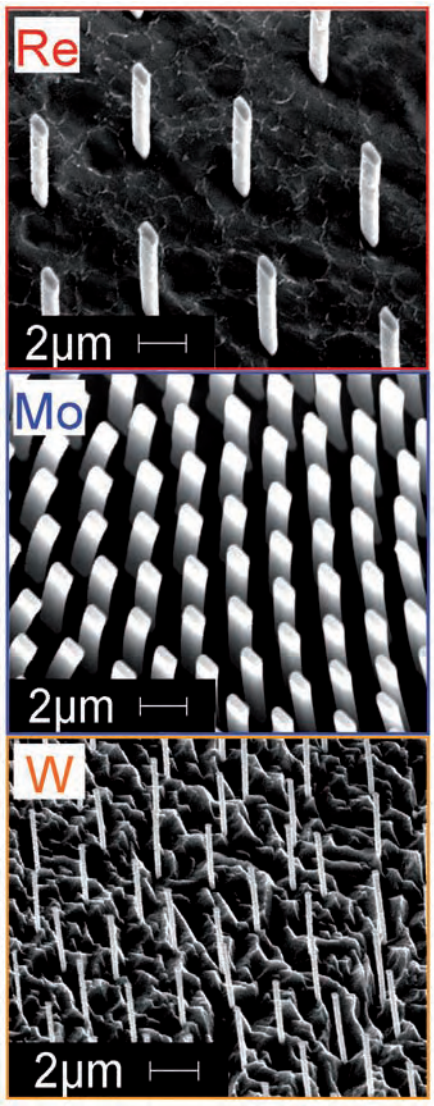

Fig. 4: *Nanowires of Re, Mo and W released from the NiAl matrix by selective etching.*

combines well-established and industrially developed techniques, thus enabling production at large scale and low costs. The feasibility of the method was demonstrated with the preparation of pseudo-binary NiAl-X (X = Re, Mo, W) eutectics (Fig. 4).

In the next step either metallic nanowires or nanopores may be produced. Metallic nanowires can be obtained from such eutectics by selective etching of the matrix.

The differences in the chemical properties, namely nobility, passivity, formation of insoluble precipitates, and kinetic hindrance of dissolution, are of great importance for the later processing of the material. The approach described here focuses on electrochemical methods for separating the phases of the *ds* materials. As a starting point for the determination of optimal electrochemical conditions for the selective dissolution of either the wires or the matrix phase the thermodynamic stability diagrams (Pourbaix diagrams) were employed [6]. These diagrams show the regions of stability for the various species (solid metal, ions of different valences, oxide and hydroxide species, etc.) as a function of the given pH and the electrochemical potential. By combining the diagrams for the individual elements it was possible to choose appropriate conditions for dissolving one phase while keeping the other phase in a passive or immune state. Fig. 5 shows such a combined Pourbaix diagram for the NiAl-W system. By choosing conditions where W is stable but Ni and Al corrode (pH 0.0, 200 mV SHE) the matrix can be dissolved while the W wires are mildly oxidized. Alternatively, choosing conditions where the matrix passivates and W dissolves (pH 6.0, 500 mV) yields nano pores in the NiAl matrix; it should be noted here that in the case of forming nano pores Al dominates

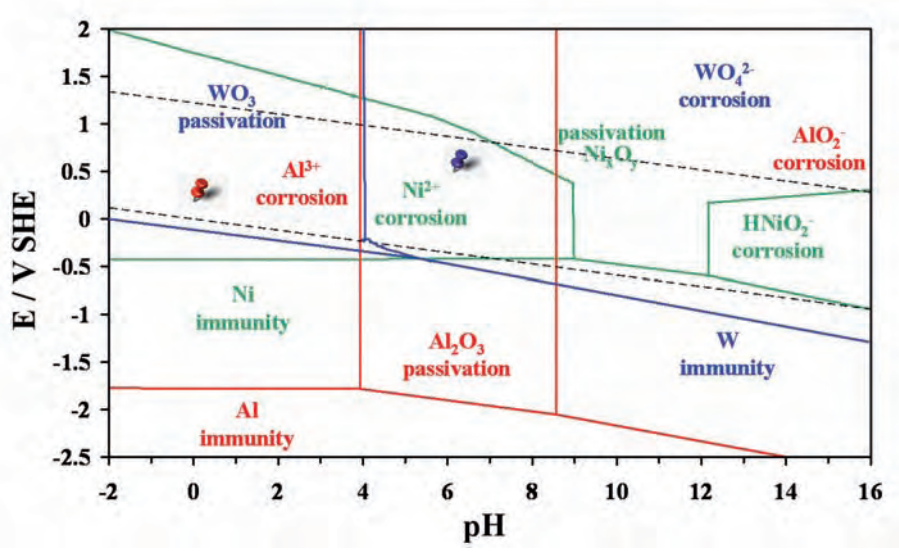

Fig. 5: *Combined Pourbaix diagram for the NiAl-W system. The red pin marks the conditions for wire exposal; the blue pin marks the conditions for pore formation.*

Fig. 6: *W nano wire tip prepared by electrochemical thinning of a directionally solidified material with subsequent cutting by a focussed ion beam.*

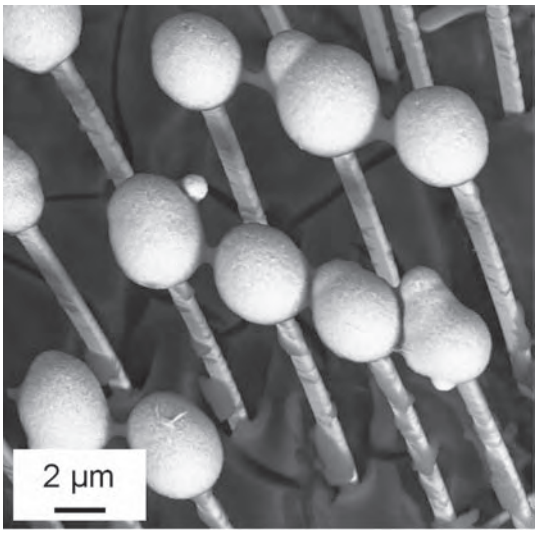

Fig. 7: *Gold semi spheres grown onto Re nanowires by electrodeposition.*

the behavior of the matrix phase allowing passivation of the NiAl phase [7].

Potential applications for these nano structures can be seen e.g. in sensor and probing technologies. The feasibility of this approach was tested by preparing a W wire rigidly embedded in and electrically contacted to a thick stem (Fig. 6). The protruding wire was then applied to the acquisition of an STM image of an HOPG test substrate.

However, this technique enables not only the formation of nanowires, but also the production of nanopores. This requires that an initial electrochemical polarisation is run under conditions which cause both the passivation of the NiAl matrix and the dissolution of the fibres (pH 6.0 for the studied systems). This procedure results in the formation of a very stable passive NiAl substrate which presents an array of nanopores uniformly distributed in its structure. The final product has a potential application as a substrate for the formation of nanosensors by electrodeposition of metals into the pores, as demonstrated by the deposition of gold in the pores left by the dissolution of Re and W fibres [8]. The NiAl-X passivation was carried out at 0.7 V for 15 minutes to allow the formation of a compact Al_2O_3 layer, with the simultaneous oxidation of Re or W to soluble species. The gold electrodeposition is subsequently done by reversing the applied current from anodic to cathodic values. The gold deposits initially grow in the pores to create gold nanowires of the same diameter as the fibrous phase present in the eutectic. The application of further pulses for the electrodeposition favours the growth of such wires on the pores, leading to the formation of gold microspheres deposited onto what remains of the Re/W wires after the polarisation pre-treatment. This can be visualised after selectively removing the NiAl phase with a mild chemical oxidation (Fig. 7). The semi spherical shape depicted by the gold deposits observed on the initial eutectics wires (Fig. 8) confirms that the electrodeposition process takes place selectively onto the fibrous phase. The dimensions of the obtained gold structures can be controlled by modification of the electrodeposition process. When the procedure is carried out in a potentiostatic mode, instead of by potential pulsing, the obtained current transients give enough information to identify the nucleation and growth processes involved in the electrodeposition. Therefore, it is possible to control the growth of gold deposits in such a manner to occur exclusively along the pores by controlling the deposition time (below diffusion controlled growth of the deposits). In this way, the formation of arrays of gold nanoelectrodes is feasible. Redox reactions carried out on this structure showed the behaviour of a macroscopic electrode demonstrating that the diffusion hemispheres on this electrode are overlapping. This should be overcome by employing the NiAl-W with its smaller nanopore diameter in which the pores are only partially filled.

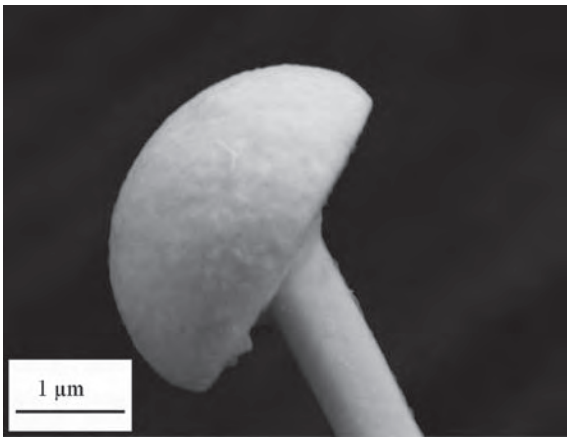

Fig. 8: *Close-up of the obtained gold deposits.*

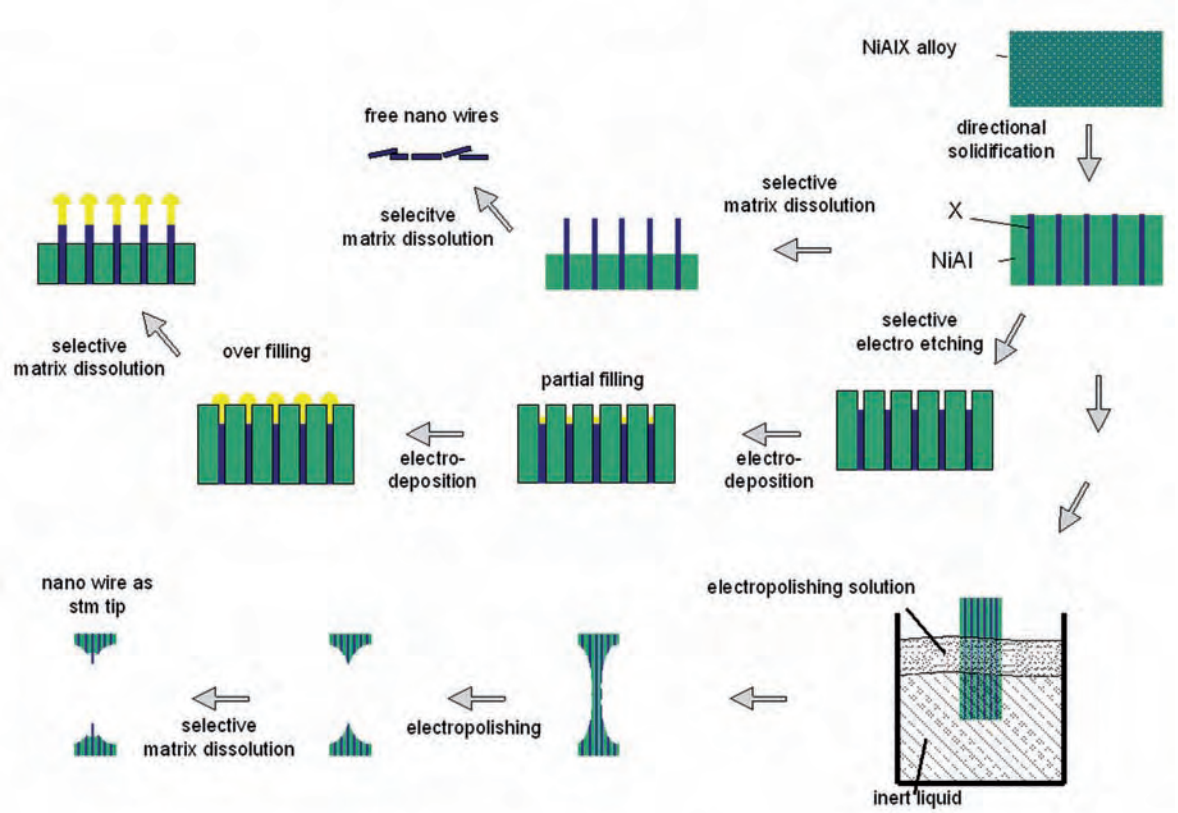

Fig. 9: *Roadmap of the different processes employed to prepare the various structures introduced here.*

Fig. 9 is a roadmap that summarizes the structures described here. After cutting a certain piece from a directionally solidified material an electrochemical step is employed in which one phase of the material is selectively dissolved in a well controlled way. This allows a tailoring of these self organised structures opening a number of possible applications such as sensors, STM tips, field emitters and basic materials for physical characterisations. This is reflected in a number of collaborations with groups in Bielefeld, Dublin, Göttingen, Heidelberg, Ilmenau, Kiel, Stuttgart, and Thun.

Acknowledgements. The financial support of the Deutsche Forschungsgemeinschaft through the projects “Production of Nanowire Arrays through Directional Solidification and their Application” and “Application of Directionally Solidified Nanowire Arrays” within the DFG Priority Program 1165 Nanowires and Nanotubes - from Controlled Synthesis to Function is gratefully acknowledged.

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3D Orientation Microscopy in a FIB SEM: A New Dimension of Microstructure Characterization

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In the present work we report our recent progress in development and optimisation of a technique for the 3-dimensional high resolution characterisation of crystalline microstructures. The technique is based on automated serial sectioning using a focused ion beam and subsequent characterisation of the sections by orientation microscopy based on electron backscatter diffraction.

Motivation: Why performing 3D investigations? Metallographic techniques for the characterisation of microstructures of materials are usually applied to study the 2-dimensional microstructure properties of a plane cut through a sample. There are, however, a large number of cases where knowledge on the 3rd dimension of a sample volume is required to understand materials properties or processes correctly. Such cases are, for example, the true size and shape of grains for grain growth investigations, the size and shape of strain fields for studies on deformation or the distribution and position of nuclei for recrystallisation investigations. An information that is completely missing in 2-dimensional microstructure observations is the full crystallographic characterisation of grain or phase boundaries including the misorientation across a boundary (this can also be determined with 2-dimensional orientation microscopy) and the crystallographic orientation of the grain boundary plane. This information is of great importance for the investigation of phase transformation or grain growth processes.

Tomography by serial sectioning. A powerful method for the 3-dimensional characterisation of crystalline materials is serial sectioning by a combination of slicing with an ion beam and EBSD-based orientation microscopy in a combined FIB (focused ion beam)-SEM (scanning electron microscope). The FIB is applied for preparation of smooth surfaces with little radiation damage by irradiation of a material surface with Ga^+ ions in grazing incidence [1-3]. By sputtering of subsequent parallel surfaces serial sections can be created with a precise distance of some 10 nm up to several µm, see e.g. [4,5]. The observation of the microstructures of the serial sections is ideally accomplished by orientation microscopy using electron backscatter diffraction (EBSD) [6-8].

The combination of EBSD-based orientation microscopy with serial sectioning is not completely new but currently under strong development as it is documented, for example, in the recent view-point set in Scripta Materialia [9] and other papers, e.g. [10-12]. Earlier publications on our work, describing a manual measurement procedure, are found in [13-15]. We have recently developed a fully automated 3D orientation microscopy system based on serial sectioning using a FIB and 2D EBSD-based orientation microscopy on a Zeiss Crossbeam FIB-SEM instrument. We expect to obtain a spatial resolution of 50 x 50 x 50 nm³ in the near future. At maximum, volumes in the order of 50 x 50 x 50 µm³ can be examined.

Principle of 3D characterisation in a FIB-SEM: Our system has been developed on a Zeiss-Crossbeam XB 1540 FIB-SEM. For EBSD a Digiview camera of EDAX/TSL is mounted on a motorised slide that allows to drive the camera computer-controlled to its position in the chamber. The geometric arrangement of the system is schematically shown in Fig. 1. In our system, in contrast to all other already available systems, the EBSD camera and EDX detector are mounted opposite to the ion column. This has the serious advantage, that, in order to change

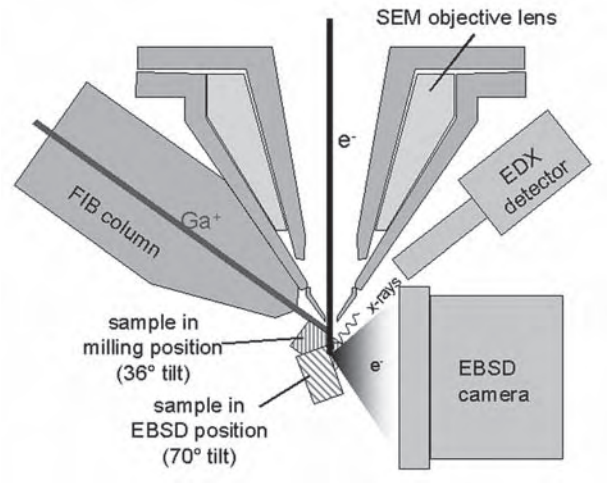

Fig. 1: *Schematic cross section through the instrument chamber, showing the sample positions for milling and EBSD analysis. To change between the two positions the sample only has to be tilted and moved in y-direction. During milling the EBSD camera is retracted to the chamber wall.*

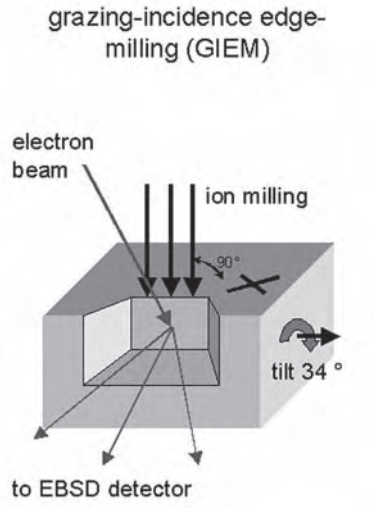

Fig. 2: *Schematics of the grazing-incidence edge milling 3D measurement procedure. The method is easy to set up and allows deep milling. The investigated area has to be at the sample edge. The black cross indicates the marker for image alignment that is milled into the sample before the process starts.*

from the milling to the EBSD position the sample only has to be moved about 2 axes which minimises possible misalignment errors. Furthermore, this set-up allows a large flexibility of the measurement set-up.

Two 3D-measurement strategies are possible. We call the first the grazing-incidence edge milling (GIEM) method, illustrated in Fig. 2: Milling is performed under grazing incidence to one surface at a sample edge. After milling has created a smooth surface in the desired distance to the sample surface the sample is moved into EBSD position by a tilt and a y movement. EBSD is accomplished on this surface. After EBSD has been finished, the sample is moved back into milling position and the next cut is performed. The method has the advantage of being easy to set-up and allowing investigation of large volume areas. In contrast, the microstructure to be investigated has to be close to the edge which is not always easily obtained or possible at all. In this case a second, alternative method may be applied, the low-incidence surface milling (LISM) method, which will be described elsewhere.

For both measurement strategies a position marker is required that allows to accurately position the sample after movement from EBSD to milling position or vice versa. As a position marker we use a cross that is milled next to the measured area into the sample surface. The marker position is precisely determined by a fully automated image processing procedure.

For the analysis of 3-dimensional data software has been developed which allows viewing any position in space of the measured volume. The software furthermore contains a tool that allows, based on manual selection of boundaries, the determination of local grain boundary normals with respect to the sample and crystal reference coordinate systems. It therefore enables access to data which can only be gained by 3-dimensional analysis.

Application example: Pearlite: Pearlite is a lamellar arrangement of ferrite (α-Fe with bcc lattice structure) and cementite (Fe_3C) that forms in a eutectoid reaction from austenite. In two-dimensional investigations pearlite often shows characteristic bending of the lamella structure which is related to a significant orientation change of the ferrite and probably also of the cementite. The latter information is not quite certain because the crystal orientation of cementite is very difficult to be measured by

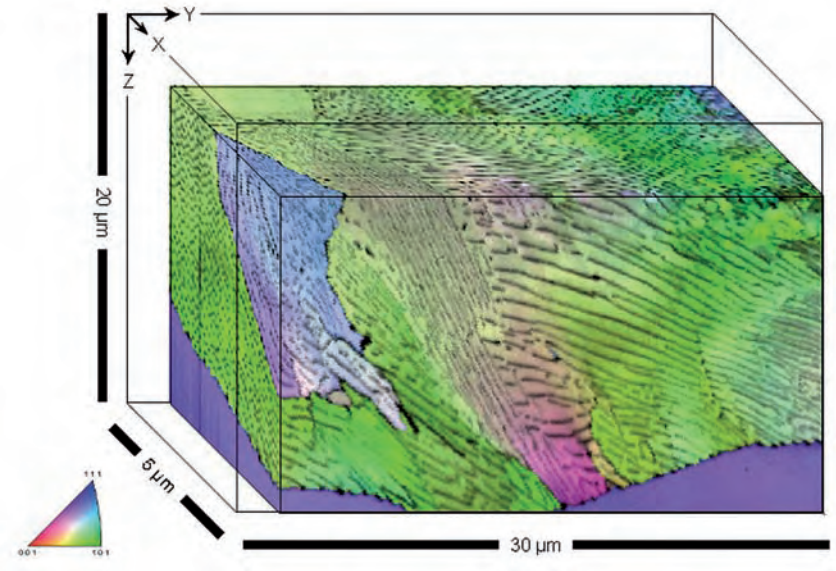

Fig. 3: *3D microstructure of a pearlite block. The colour is composed by image quality (grey value) and a colour code for the crystal direction parallel to the X-axis of the sample. The outer block indicates the full measured volume. A part has been cut off because of low pattern quality in these areas.*

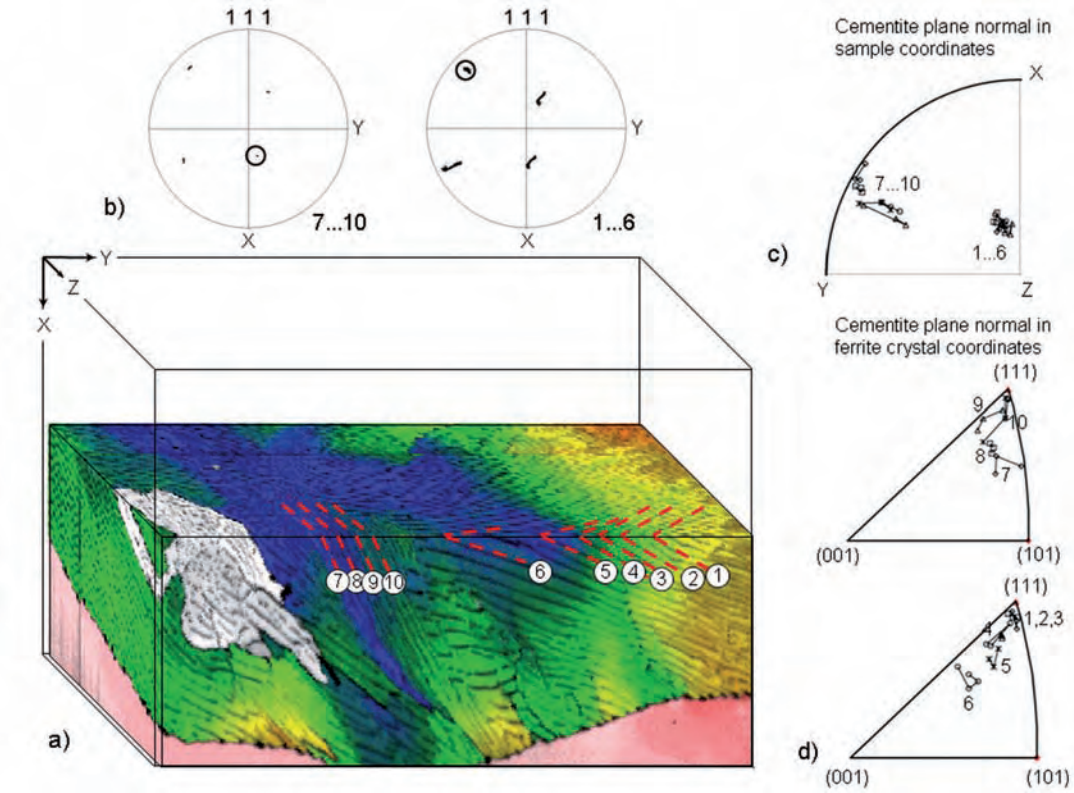

Fig. 4: *Ferrite-cementite interface analysis. a) Microstructure with some cementite lamellae marked. b) (111) pole figure of the area of lamellae 7 to 10 (left) and 1 to 6 (right) indicating that each pearlite colony is characterised by one common (111) pole as rotation axis. The common pole is marked by a circle. c) Stereographic projection of the cementite lamellae plane normals. d) Inverse pole figure of the crystallographic ferrite plane normals of the cementite lamellae. For both colonies ferrite plane normals close to (111) are found, though with a significant deviation. For figures c) and d) each lamella position has been measured several times indicated by similar symbols, connected by lines.*

electron diffraction techniques due to its low structure factors. The occurrence of bending and of the related orientation change is an interesting hint on the physical mechanism of phase transformation. Several models have been put forward to explain the pearlite formation, e.g. [16,17]. A 3-dimensional investigation of the arrangement of pearlite lamellae yields a number of new and otherwise not obtainable information that may help to determine the correct mechanism: first, the direction of maximum orientation gradients may be determined and spatially correlated with the strength of lamella curvature. Second, the ferrite-cementite phase boundary might be precisely characterised for example in terms of the ferrite grain boundary normal.

For 3D investigations a simple high carbon steel Fe-0.49% C sample has been taken. The sample was heated to 950°C and then furnace cooled with 0.1°C/s. The measurement system was set up for a GIEM measurement. 50 slices were milled with a step size of 100 nm. On each slice orientation mapping was performed on an area of 30 x 20 µm² using a lateral step size of 100 nm as well. The time for one complete cycle was about 35 minutes including 16 minutes of milling and 15 minutes of EBSD mapping.

Fig. 3 displays the result of the measurement in form of a 3D orientation map. The figure displays a map where the colour of each voxel (volume pixel) is composed by an overlap of the diffraction pattern quality which defines the brightness of the voxel and the orientation of the measurement plane normal given in an inverse pole figure colour triangle. Though cementite could not be indexed, the diffraction pattern quality indicates the position of the lamellae by a reduced pattern quality. The figure shows the high alignment accuracy of the measurement: in the third dimension the eye is at many positions able to follow the pearlite lamella.

One of the most significant advances of 3D orientation microscopy compared to the 2D technique is the possibility to determine grain or phase boundary planes. Currently a semi-automatic tool is applied to measure the position of boundary planes. From 3 user-defined points on a plane the plane normal vector with respect to the sample and crystal coordinate system is calculated. The results are demonstrated in Fig. 4. Two sets of pearlite lamellae, 1 to 6 and 7 to 10 have been investigated. As indicated by the pole figures in Fig. 4 b, in each of the lamellae groups the ferrite crystals continuously rotate about a specific (111) pole which is different

for both groups. The position of the lamellae normals in sample coordinates is displayed in the pole figure in Fig. 4c. The crystallographic indices of the ferrite side of the lamellae boundaries is shown in the inverse pole figures in Fig. 4d. The cementite side cannot be indexed since the orientation of cementite could not be determined. The inverse pole figures show, that the ferrite phase boundary is close to (111) with, however, a significant deviation of up to 16°. This deviation is only to a minor part due to measurement inaccuracies, i.e. inaccuracies of spatial measurement and orientation determination. It has been shown by TEM investigations that the atomic habit plane of ferrite-cementite lamellae may be (215), (112) or (101) (see [18,19], for example), depending on the orientation relationship between both phases. The (111) plane determined here is quite far off of these results but it has, in fact, been shown that there is not necessarily any correspondence between the atomic habit plane and the macroscopic one [20]. From the present results it seems, furthermore, that there is also no clear relationship between crystal orientation and macroscopic habit plane.

Conclusions. A system for 3-dimensional orientation microscopy based on fully automated serial sectioning and EBSD-based orientation microscopy has been developed in a FIB-SEM. The technique yields a multidimensional data vector for each voxel of the measured volume, including the crystal orientation, the crystallographic phase and a value for the lattice defect density. A volume pixel resolution of 100 x 100 x 100 nm³ has been obtained as a standard, but 50 x 50 x 50 nm³ seems to be a realistic optimum. The largest volumes observable are in the order of 50 x 50 x 50 µm³. The technique works on a large number of materials but some exceptions have been found. In particular, metastable austenite occurring in various steels seems not to be accessible by the technique because it transforms into ferrite under Ga^+-ion beam irradiation.

In comparison to newly developed 3D x-ray diffraction techniques the 3D orientation microscopy technique has the advantage of a significantly higher spatial resolution, applicability also to highly deformed or multi-phase structures, and ease of application. A serious disadvantage is the fact that the technique is destructive, that means that a volume that has once been investigated is destroyed and in-situ studies are principally impossible. The two techniques appear largely complementary rather than being in direct competition.

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Observation of a Honeycomb Structure in the Twisted Plywood Mesostructure of a Chitin-Based Fibrous Biological Nano-Composite Tissue

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Many fibrous biological nano-composite tissues based on chitin, collagen, or cellulose reveal a high degree of hierarchical organization, Fig. 1 [1]. The most characteristic feature of such materials are mesoscale structures which are referred to as Bouligand- or twisted plywood patterns, Fig. 2 (next page) [2]. According to earlier work [3-7] these structures consist of helicoidal stacks of planar fibrous polysaccharide-protein arrays (Fig. 1). The thickness of one such layer corresponds to a certain stacking sequence of planes which are gradually rotated about their normal axis. This study reveals that this picture of the inner structure of fibrous biological tissues must be refined. Our experiments on the cuticle of the large arthropod *Homarus americanus* (lobster) show in particular that the plywood structure reveals a more complex internal order of its constituent fibers and planes than commonly assumed.

The cuticle of lobster consists of the three main layers epicuticle, exocuticle, and endocuticle (Fig. 2). The epicuticle (outer skin) is a thin waxy layer which acts as a diffusion barrier. The exocuticle and endocuticle layers carry the mechanical loads. They consist of a hard fibrous chitin-protein tissue containing calcium carbonate minerals (typically crystalline or amorphous calcite) of nanoscopic size [8,9]. It are these two layers (exocuticle and endocuticle) which reveal the Bouligand structure [3-7]. For microstructure characterization (OM, SEM, TEM) specimens for this study were cut from the dried left cheliped (crusher claw). Details on sample preparation can be found in [4-6].

In accordance with earlier studies Fig. 2 shows that the tissue of the exo- and the endocuticle of *Homarus americanus* reveals two main microstructural scales.

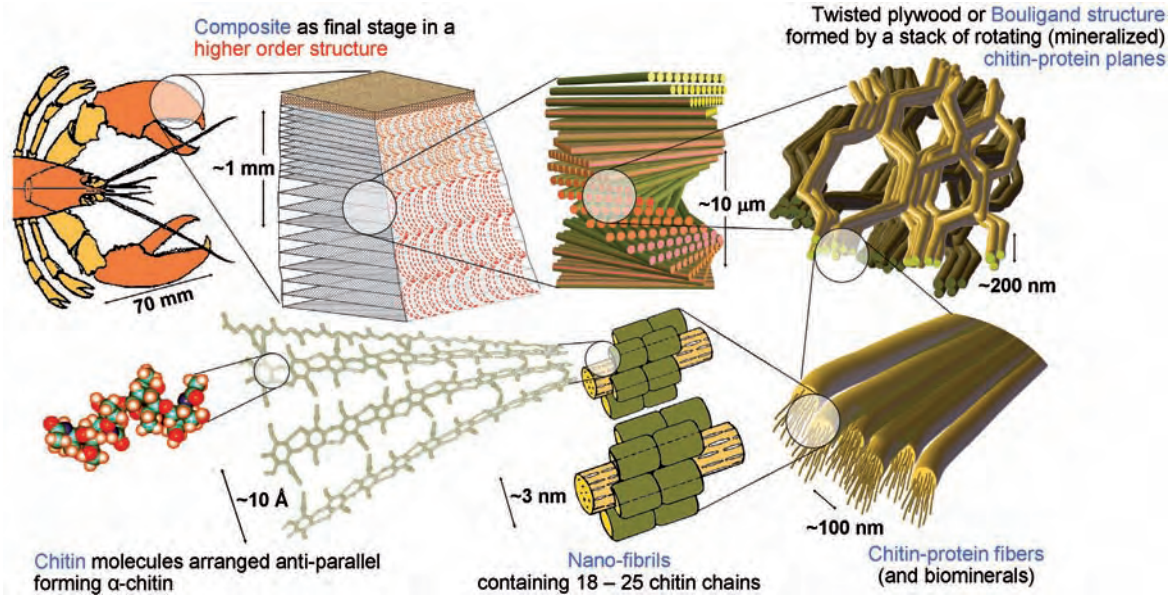

Fig. 1: *Structure of the exoskeleton material of Homarus americanus. A characteristic feature of the material is its hierarchical organization. It reveals six main structural levels: The first level is the polysaccharide molecule (chitin). Its antiparallel alignment forms α-chitin crystals. The second level is the arrangement of 18 to 25 of the polysaccharide molecular chains in the form of narrow and long crystalline units, which are wrapped by proteins, forming nanofibrils of 2-5 nm diameter and 300 nm length. The third level is the clustering of such fibrils into chitin-protein fibers of about 50-300 nm diameter. The fourth level in the hierarchy is the formation of a woven network of such chitin-protein fibers (Fig. 2). The spacing between them is filled by proteins and clusters of calcite. The fifth level, visible in optical microscopy, is referred to as twisted plywood or Bouligand pattern. This level is created from the woven chitin-protein planes. Their gradual rotation from one plane to the next creates complex structures (sixth level) which appear as fibril arches when viewed in cross sections (Fig. 2).*

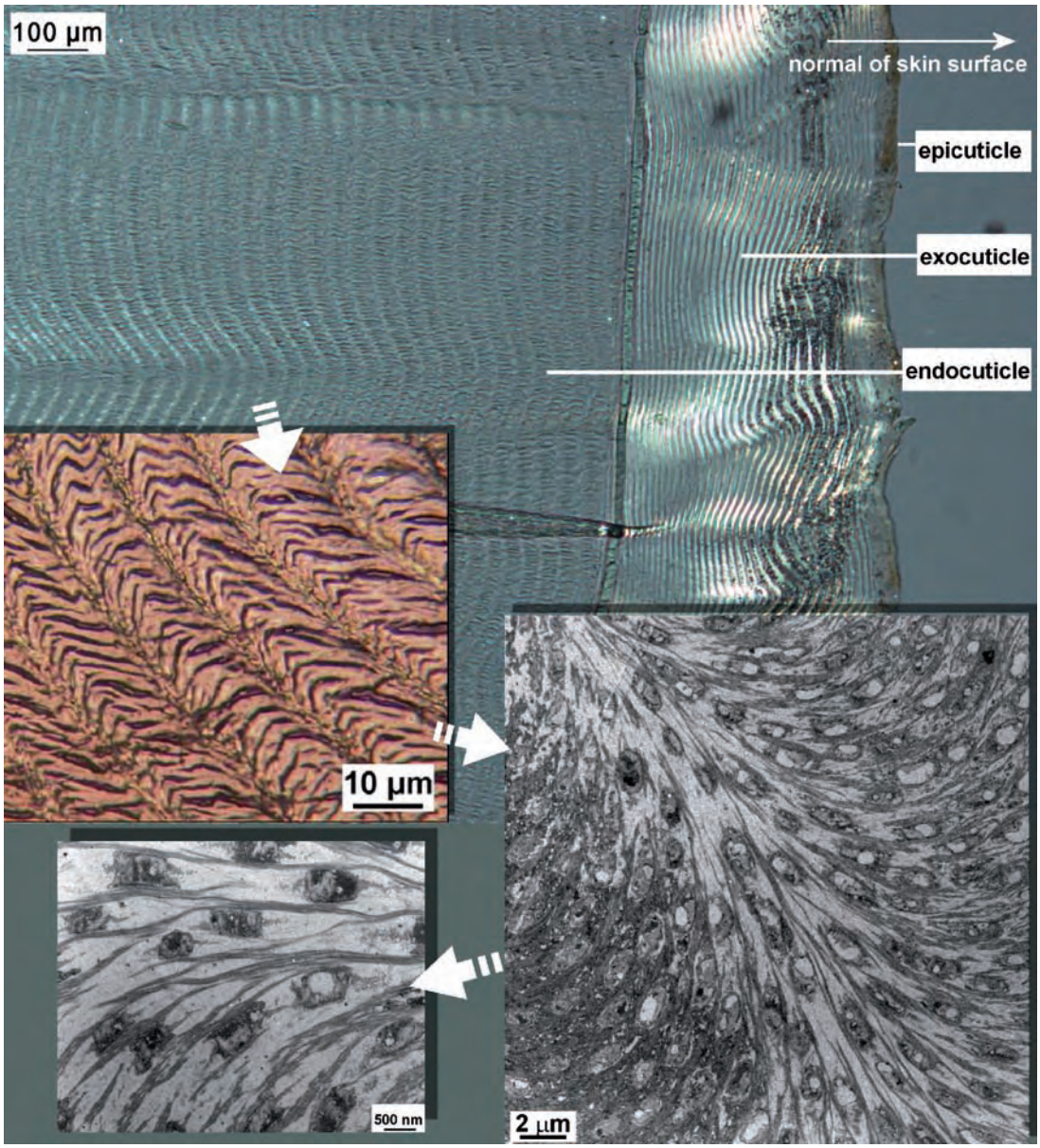

Fig. 2: *Microstructure hierarchy in the exoskeleton of the lobster Homarus americanus. The images were taken by optical and electron microscopy. The micrographs reveal the hierarchical organization of the material particularly inside the twisted plywood pattern.*

At the mesoscale (optical resolution) the matrix shows a twisted plywood pattern, which is characteristic of the cuticle of arthropods [3-7]. From the electron micrographs we can confirm that this Bouligand-type matrix is itself formed by stacks of mutually misoriented chitin-protein fibril planes which contain embedded biominerals, Figs. 1, 2. The microfibrils in these planes, which appear in dark gray in the electron micrographs, have a diameter of about 50 to 300 nm. Each of these microfibrils consists itself of a bundle of parallel nanofibrils which contain the actual polysaccharide molecular chains wrapped by proteins, Figs. 1, 2.

A *quantitative* microscopical study of the inner structure of the Bouligand pattern is difficult though owing to the influence of stereology. This means that the appearance of the patterns depends on the angle at which the sample was cut. Therefore, we decided to apply synchrotron wide angle x-ray diffraction for a more detailed study of the arrangement of the nanofibrils within the mesostructure. The advantage of this approach is that the nanofibrils are crystalline, i.e. the polysaccharide molecules arrange in the form of the α-chitin phase which assumes an orthorhombic crystal structure with the lattice parameters a = 4.74 ± 0.02 Å, b = 18.86 ± 0.01 Å, c = 10.32 ± 0.04 Å [10]. Furthermore, the elongated crystalline arrangement of the molecules within the nanofibrils means that their *crystallographic* orientation distribution reflects also the *topological* orientation distribution of their longitudinal axis. Only when discussing rotations of the crystalline nanofibrils

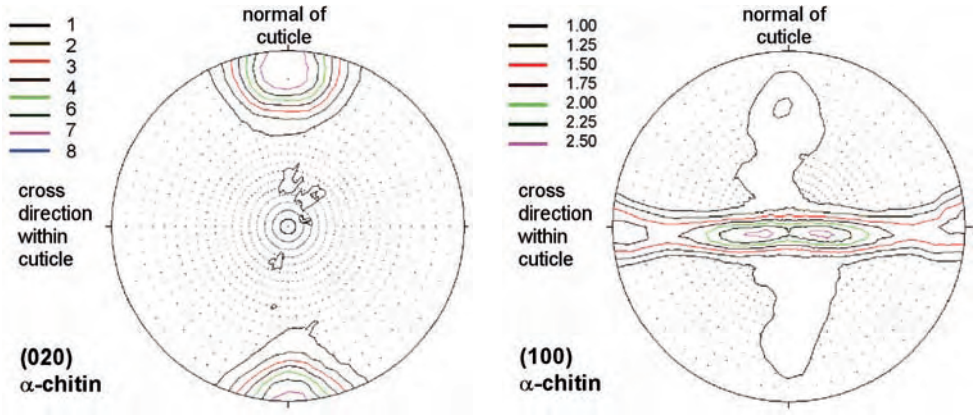

Fig. 3: *Pole figures of the α-chitin fiber network within the Bouligand structure measured in the claw of Homarus americanus by using synchrotron radiation; 2 x 5 mm sample section; 1 x 1 mm beam size; rectangular sample shape. The reference coordinate system for the two projections are the top (plane surface) and in-cuticle transverse directions of the claw, respectively. The wavelength amounted to 0.196 Å.*

about their common longitudinal axis one has to carefully distinguish between the crystallographic and the topological orientation.

The measurements were carried out at the synchrotron source at HASYLAB / DESY (Germany). We used a monochromatic beam with a wavelength of 0.196 Å in wide angle Bragg diffraction mode. An area detector was used for the measurement of Debye-Scherrer frames from which texture-corrected theta scans for phase analysis and pole figures for texture analysis were obtained. Fig. 3 shows the two pole figures, {100} and {020}, after correction and normalization. The reference system of coordinates for the projection of the two pole figures is the normal direction of the claw surface (upper direction in the pole figures) and the transverse direction within the cuticle cross section.

Fig. 3a shows that the texture of the nanofibrils is characterized by a very strong fiber texture with a crystallographic <020> axis parallel to the surface normal axis of the cuticle. This means that the b-axis (*long axis of the lattice cell*) of the α-chitin crystals points towards the surface of the exoskeleton within an orientation spread of about 15°. It must be emphasized that such a strong crystallographic texture is very uncommon even in man-made materials. Such a strong preferred orientation distribution of the nanofibrils could not be expected from the micrographs shown in Fig. 2.

A second important outcome of the orientation data ({100} pole figure in Fig. 3b) is that the occupation of the <020> fiber texture is not isotropic but shows two pronounced maxima of the {100} peaks which are misoriented by about ±25-30° and two weaker

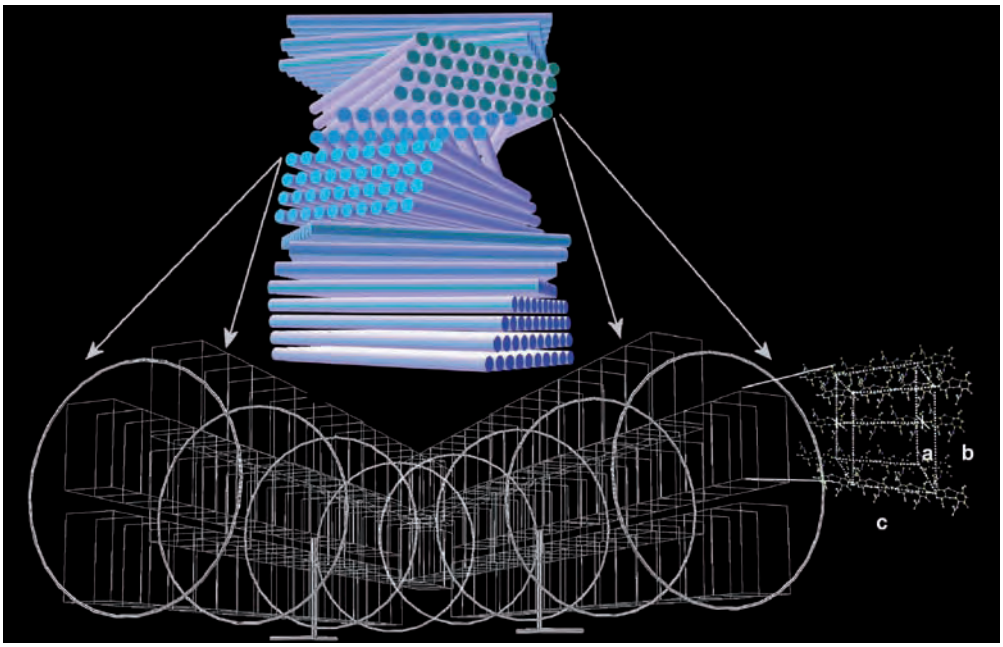

Fig. 4: *Schematical drawing of the main texture components of the chitin nanofibrils in the Bouligand structure.*

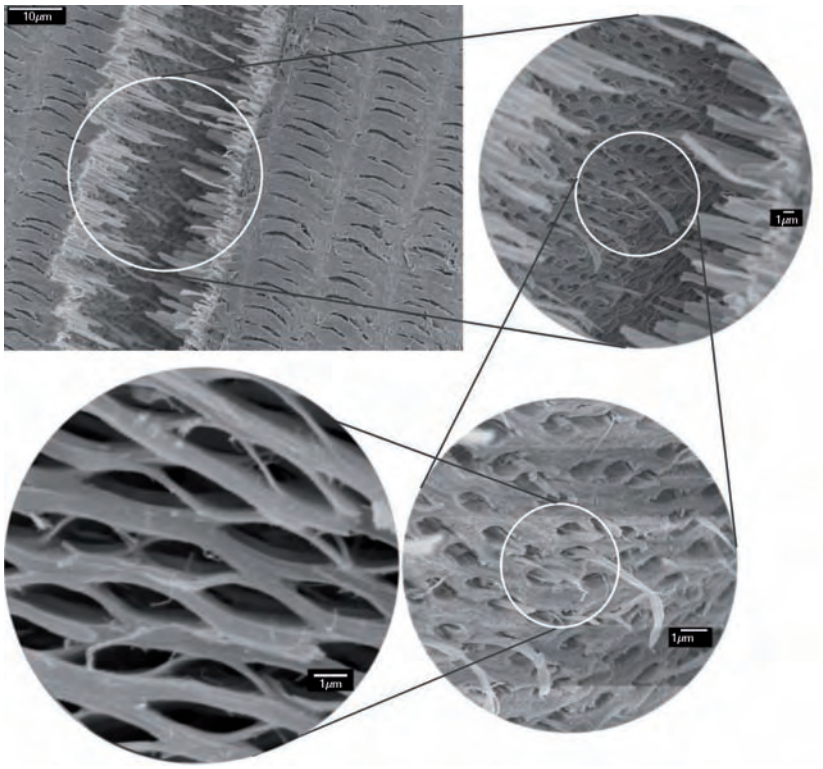

Fig. 5: *Electron micrographs (SEM) taken from fractured specimens of Homarus americanus. The images underline the important role of the woven inner hierarchy of Bouligand structured material.*

maxima which are misoriented by about ±85-90° from the pole figure center within the equatorial plane. This means that the chitin-protein fibers do not only have a common <020> axis pointing at the cuticle surface but also two major and two smaller preferred crystalline branches within the cross section of the network, Fig. 4. This observation resembles earlier results which were reported by Weiner et al. [11] on preferred topological orientations (30° and 70°) which they found in twisted plywood arrangements of the collagen fibril arrays in primary lamellar bone of rat. When comparing the texture measurements (Fig. 3), particularly the preferred angles close to 30° and 90° in the cross section plane, with the micrographs shown in Fig. 5 it becomes obvious that the chitin-protein fibers are arranged in the form of a honeycomb structure.

Following earlier investigations on the nature of the excellent fracture toughness typically reported for fibrous biological nanocomposites [12] two main reasons are conceivable for the occurrence of such a pronounced crystallographic and topological texture of the chitin-protein fibers. The first one is the possibility of an enhanced resistance against crack propagation created by such microstructures: One may speculate that an orientational discontinuity in the stacking sequence of the mutually misoriented chitin-protein planes has advantages for crack path deflection or crack branching as opposed to a smooth orientational transition from plane to plane which would be less suited to impede crack propagation. Second, the chitin planes do not simply consist of parallel bundles of nanofibrils but of planar honeycomb-type arrays of fibers which are penetrated by equivalent planar structures under some oblique angle, Fig. 5. This type of arrangement provides a very high density of interfaces which have to be critically stressed against frictional forces upon fiber pull-out. Such a mesh of two (or more) interpenetrating planar honeycomb-type structures should provide a very high mechanical stability against fracture initiation and propagation.

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Creep Damage Investigation by Combined Synchrotron X-ray Diffraction and Tomography

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The efficiency of electricity-generating power plants and gas turbines depends strongly on their components' sustainability of loading at high temperatures. The service lifetimes of these components is controlled in most cases by creep-induced cavity growth during tertiary creep. In many technical applications such as stationary power plants and aero-engines knowledge about the remnant lifetime of creep-loaded components is crucial for a safe and cost-effective operation.

So far creep damage could only be determined from two-dimensional microscopy images of microstructure sections. Thus only snap-shots of the damage evolution were available. Compared to such microscopy, synchrotron x-ray tomography has the advantages of providing data of damage in the bulk, which often differs substantially from damage at the surface [3], and the continuous recording of data allows for revealing the evolution of damage locally as a function of time.

In principle both diffraction and tomography can be performed using monochromatic or white X-rays. Due to the higher photon flux compared to monochromatic high energy X-rays, the white beam allows substantially faster data acquisition. However, the spatial resolution at the currently available white beamlines is at best 1.5µm x 1.5µm x 1.5µm, and thus an order of magnitude lower than the resolution available in standard experiments using monochromatic radiation, i.e. 0.3µm x 0.3µm x 0.3µm. Tomography experiments using white high energy synchrotron radiation, thus, appear advantageous for following the kinetics of processes such as crack growth, sintering processes or creep damage.

While both diffraction and tomography experiments are well established techniques, only recently both methods were combined within one experiment [2] due to the challenges in choosing an effective compromise e.g. in the beam properties, in the alignment of the increased number of components of the experimental set-up with the high precision required, and in using different detection systems simultaneously.

The experiments were carried out at beamline ID15A of the ESRF [4]. The experimental set-up consisted of three detection systems, which allowed us to perform tomography, energy-dispersive diffraction and angle-dispersive diffraction without further alignment or calibration procedures during the experiment (Fig.1). Tungsten carbide slits defined the gauge volume within the sample.

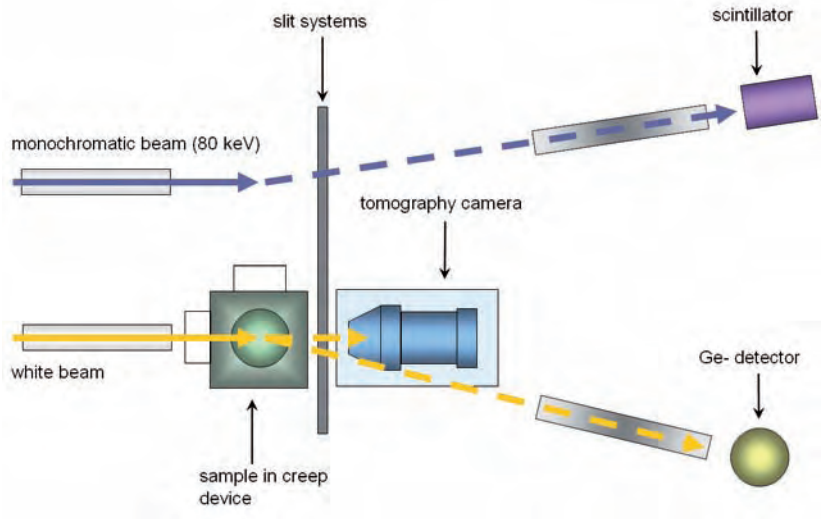

Fig. 1: *Experimental set-up of a combined diffraction/tomography experiment using both the monochromatic beam for diffraction and the white beam for tomography.*

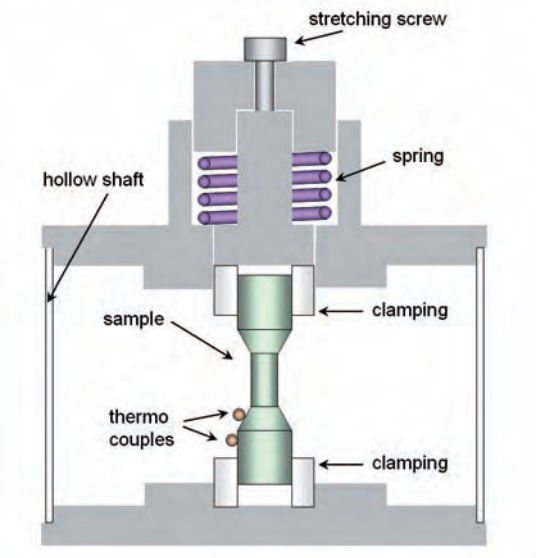

Fig. 2: *Miniaturized creep device developed at TU Berlin.*

In order to investigate creep damage evolution in-situ by both synchrotron X-ray diffraction and tomography, a miniaturized creep device (Fig. 2) was developed at TU Berlin.

In these experiments we investigated the brass alloy CuZn40Pb2 (~58 wt.-% Cu, 40wt.-%Zn and 2wt.-% Pb), which contains three phases: α-brass, β-brass and Pb. The Pb shows a strong absorption contrast to both brass phases. By identifying the location of selected Pb particles within slices perpendicular to the sample axis, we could follow the damage evolution in defined sub-volumes of the sample as a function of creep time. In order to provide the conditions for as realistic a creep experiment as possible during the limited beamtime available, the sample was deformed in tension (4.47% in total) prior to the creep experiment according to the results given in [5].

Tomography revealed that in the initial state, after 4.47% prestraining – but before the creep test – the hot-extruded samples contain small mostly spherical or ellipsoidal voids. The latter voids are elongated in the stress direction. During creep additional voids nucleate and their number and size increases with increasing creep time (Fig. 3), see [2] for more quantitative results.

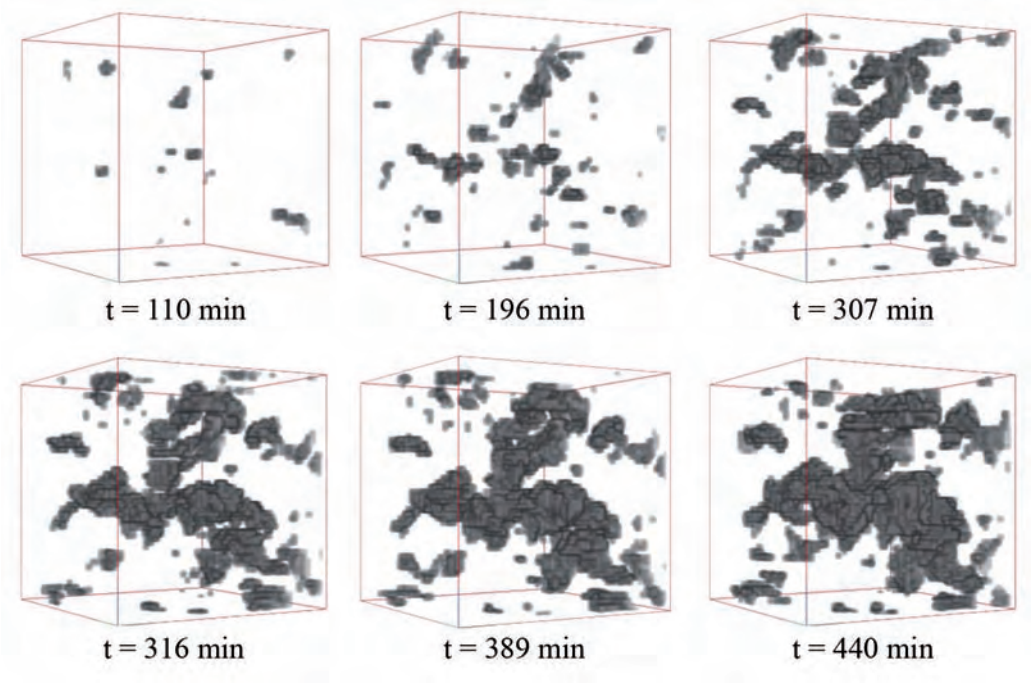

Fig. 3: *Void evolution (black) during creep of CuZn40Pb2 at 375°C under 25MPa tensile stress (size of the shown sub-volume: 80µm x 80µm x 80µm,spatial resolution: 1.5µm x 1.5µm x 1.5µm).*

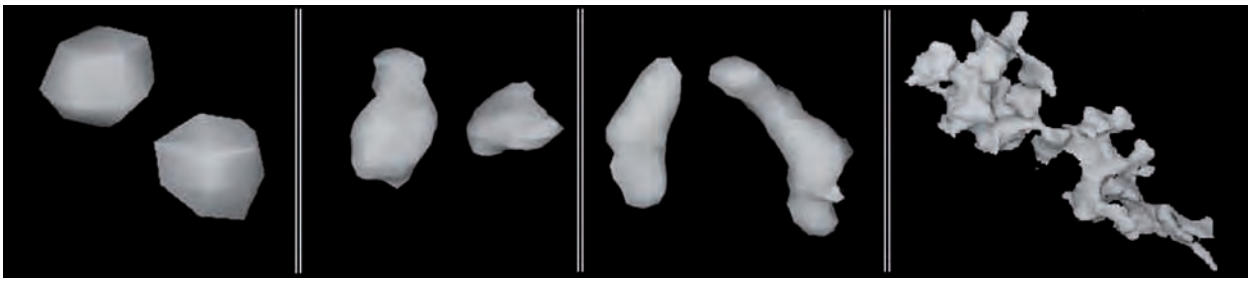

Fig. 4: *Typical void shapes: sphere-like, ellipsoid-like, rod-like and irregular.*

The morphology of the possible void shape changes from globular, i.e. nearly spherical, ellipsoidal or rod-like to irregular shapes is illustrated in Fig. 4. The change in morphology is due to void growth and void coalescence in particular at grain boundaries that are perpendicular to the load axis. In order to characterize the orientation of the voids with respect to the stress axis, the voids were represented by equivalent ellipsoids of equal volume and moments of inertia.

The orientations of the longest axis of these ellipsoids with respect to the stress axis change from parallel to perpendicular during the creep test (Fig. 5). This is presumably due to void growth and coalescence along respective grain boundaries in the later stage of the creep test.

The diffraction data revealed the formation of texture complying with the typical tensile test <111>/<100>-fibre texture of fcc α-brass after about 296 min creep time.

Acknowledgements: The authors acknowledge the support of Ms. A. Pernack, TU Berlin, Germany, Dr. T. Buslaps and Dr. M. di Michiel, both ESRF Grenoble, France, in performing the combined diffraction/tomography experiment and the support of Mr. Dipl.-Ing. A. Kottar, TU Wien, in software development for quantitative creep damage analysis. The authors thank Dr. H.M. Mayer for the tensile deformation of the samples prior to the creep experiment, Mr. Dipl.-Ing. B. Breitbach, MPIE, for drawing the figures of this chapter, D. Fernandez-Carreiras of ESRF for the imaging detector control system and the ESRF for beamtime at ID15A and financial support of travelling expenses. A.P. and W.R. also gratefully acknowledge the Deutsche Forschungsgemeinschaft (DFG) for financial support of the project Py9/1-2.

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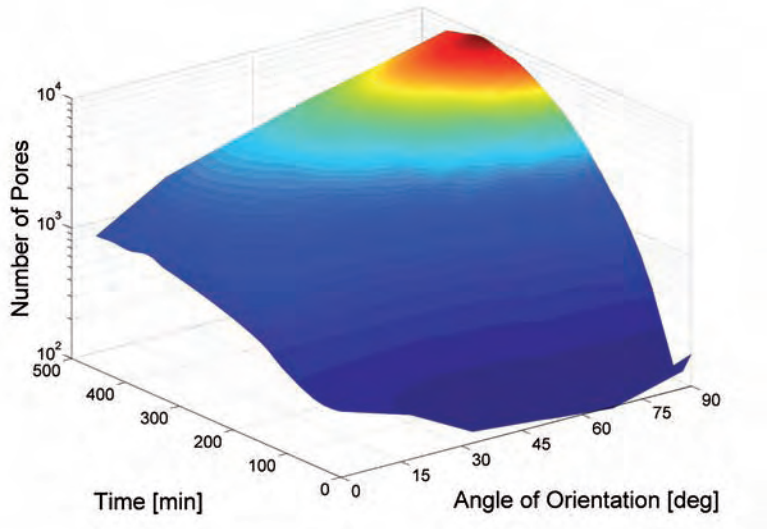

Fig. 5: *Void orientation distribution (as characterized by the angle between long void axis and stress direction) as a function of creep time.*

Ab-initio Based Multiscale Calculations of Grain Boundaries in Aluminum

L. Lymperakis, J. Neugebauer

Department of Computational Materials Design

Introduction. Grain boundaries (GBs) are the central structural features in thermomechanical processes such as recovery, recrystallization, and grain growth and significantly affect the physical and mechanical properties of materials. Grain boundary engineering, i.e. optimizing the population of GBs with desirable geometry by suitable thermomechanical treatment, is nowadays an important topic in functional and structural materials design [1-3]. To achieve this, a deeper understanding and quantification of the the GB energies with respect to the misorientation of the two grains (3 dimensional phase space) and the inclination of the boundary plane (2 dimensional phase space) are crucial.

Methodological aspects. Extended defects such as dislocations and GBs impose the challenge of treating different length scales: The core structure of the defect is rather localized, while the strain field introduced by the defect may be significant even far away from the core. In order to tackle this problem we have generalized our Implicit Boundaries Multiscale Scheme (IBMS) approach which had been originally developed and applied to study isolated dislocations [4]. The IBMS combines elements of *ab-initio* calculations, empirical potential calculations and elasticity theory and bridges the microscopic with the macroscopically relevant length scales associated with extended defects. *Ab-initio* based methods are a reliable tool for atomic scale calculations and thus suitable to describe the highly distorted defected area of the material. However, they are characterized by a rather limited (limited by the available computational power) ability to describe systems consisting of large numbers of atoms. On the other hand, empirical potentials are suitable for describing elastically strained or bulk like regimes consisting of more than 10^5 atoms. Within the IBMS approach the different regimes are linked utilizing implicit boundaries. The accuracy of this approach is in principle limited only by the accuracy of the *ab-initio* calculations. In principle, the IBMS approach can be applied in any system which can be modeled with a supercell geometry containing a pair of defects which are separated by elastically strained or bulk like material.

In this work we use the IBMS approach to study (GBs) in Aluminum: in order to describe the highly distorted material close to the boundary region we perform total energy and force Projected Augmented Wave (PAW) method calculations [5] while the PBE-Generalized Gradient Approximation (GGA) [6] is used to model exchange and correlation. Modified

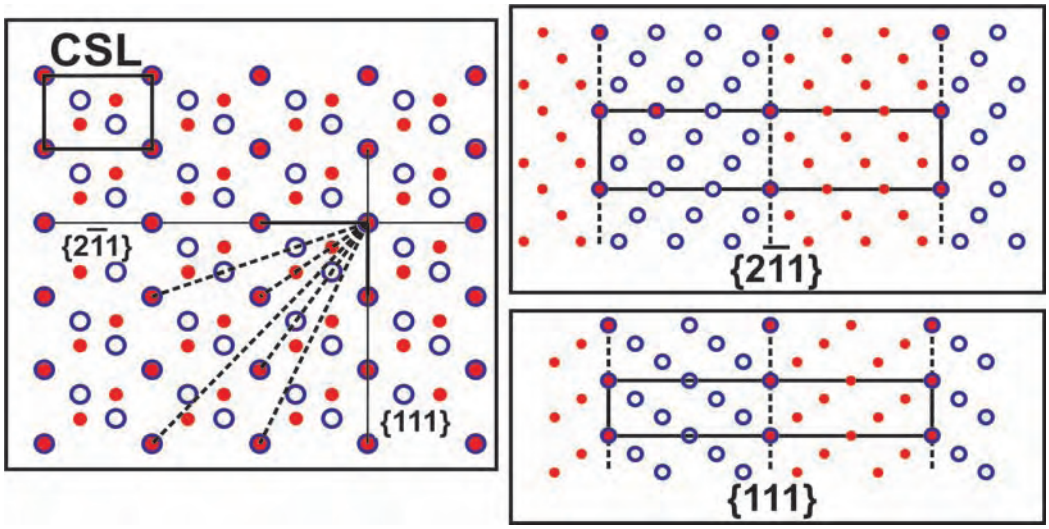

Fig. 1: *Left part: Moiré pattern of the Σ3 CSL. Open and filled circles denote the lattices of the two grains. The coincidence points of the two lattices form the CSL. The thin straight lines parallel to the {111} and {2$\bar{1}$1} directions denote the primitive vectors of the CSL. The dashed lines which pass through points of the CSL correspond to inclined planes of the Σ3 GB. Right part: Supercells corresponding to the {2$\bar{1}$1}Σ3 and {111}Σ3 GBs. Each supercell contains a pair of defects denoted by the dashed lines. The distance between them can be varied in a discrete manner by choosing different planes of the CSL to the left.*

Embedded Atom Method (MEAM) calculations are used to describe the elastically strained bulk like material between the boundaries [7]. The supercells contain a pair of boundaries to set the total dislocation dipole to zero. In order to construct supercells with a pair of GBs the Coincidence Site Lattice (CSL) [8] approach is used: For each Σ value different planes of the corresponding CSL correspond to different misorientation and/or inclination angles (see Fig 1). Thus, the whole range of misorientation and inclination angles may be assessed in a discrete manner by choosing various CSLs and various CSL planes. Furthermore, any two parallel CSL planes correspond to two identical GBs. Thus, for each misorientation and inclination angle different supercells containing GBs with different separation distance are constructed. The great advantage of our approach is that due to the periodic boundary conditions the boundary area is kept fixed for each GB calculation. Thus, the possibility of the boundary plane to reconstruct according to the Wulff-Herring reconstruction [9,10] is rather limited and in principle GBs with the exact assumed misorientation and/or inclination are calculated.

Results. In a first step we focused on symmetrical tilt GBs having rotation axes parallel to the high symmetry <110>, <111>, and <100> directions of the fcc lattice. Thus, we sequentially explore the three degrees of freedom associated with the misorientation of the grains. In Fig 2 the energies for symmetrical tilt <110> GBs are shown along with GB Character Distribution (GBCD) data from recent experimental report by D. M. Saylor *et al*. [11]. As revealed by Fig 2, GBs of low index and low Σ value exhibit low energies. Thus, it is expected that for conditions close to thermodynamic equilibrium which are usually accessed during thermomechanical treatment processes, these GBs will have the largest populations. Indeed the GBCD line shown in Fig 2 follows an inverse relationship with respect to our calculated energies. Furthermore, our results closely reproduce previous experimental assessed GB energies for <110> and <100> symmetrical tilt GBs in Al [12].

In a second step we extend our search to the remaining two degrees of freedom associated with the boundary plane orientation. We focus on the technologically interesting low-energy/low-Σ GBs and we calculate the energies for various, normal (vertical inclinations) and parallel (horizontal inclinations) to the rotation axis boundary inclinations. This approach allowed for the first time an atomistic description of the two degrees of freedom associated with GB inclinations. The results for the Σ3 horizontal inclinations are shown in Fig 3. Since a reconstruction of the inclined interface does not require a change in the grain texture, a Wulff-Herring-like reconstruction is more likely to occur here. A comparison of the calculated energies with the predicted Wulff-Herring reconstruction energy reveals the interplay between kinetics and thermodynamics and shows the strong tendency of the inclined planes to reconstruct to lower energy planes on the expense of increasing the boundary area.

Discussion and conclusions. In this work the 5D space of GBs in Al has been systematically explored applying our IBMS approach. Our calculations confirm the empirically established tendency of low Σ value and low index GBs to exhibit low energies. Moreover, they reveal a strong tendency of plane

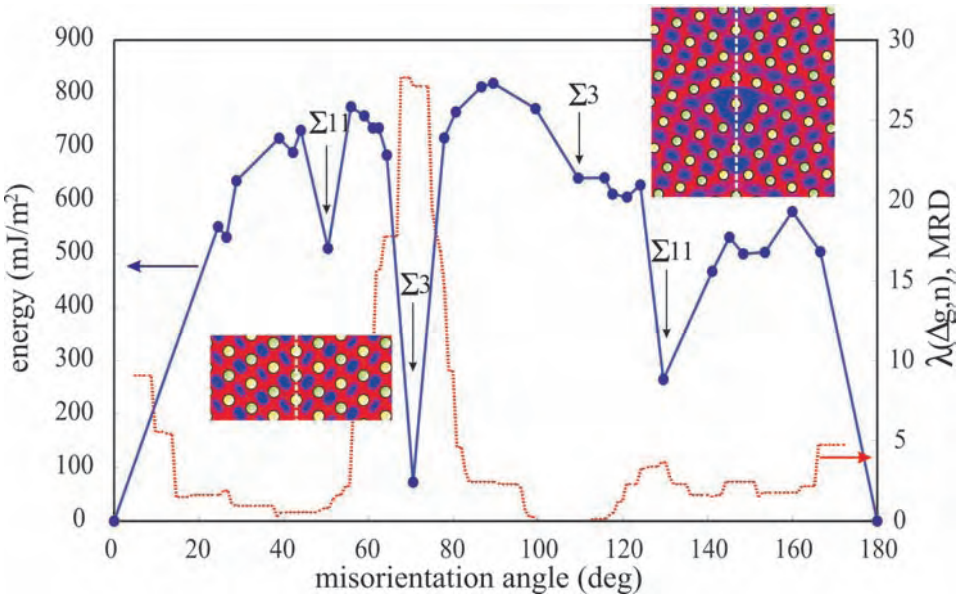

Fig. 2: *Formation energies (solid blue line) of the <110> symmetrical tilt GBs in Al. The grain boundary character distribution GBCD (dotted red line) measured experimentally [11] is inverse proportional to the calculated energy (see text). Insets: Total charge density distributions around the boundary plane for the* {111}Σ3 *(left) and* {2$\bar{1}$1}Σ3*(right) GBs. The strong interatomic cohesion at the interface at the* {111}Σ3 *is clearly depicted.*

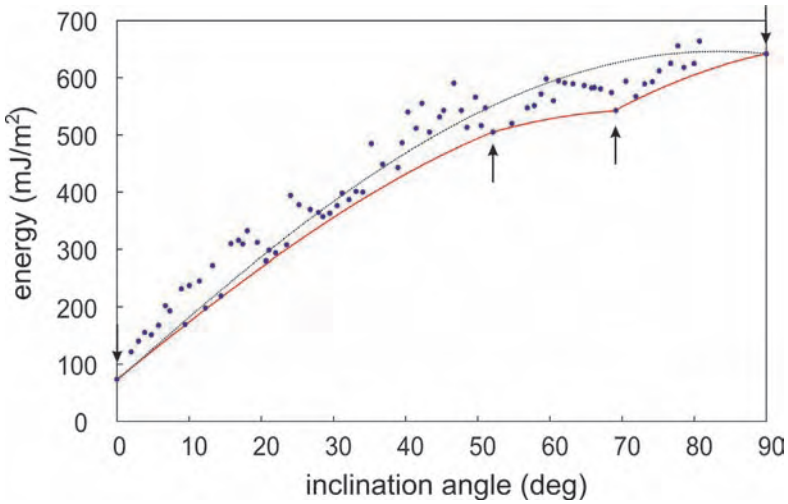

Fig. 3: *Boundary energies as function of the horizontal inclination angle for the Σ3 GBs. The point indicated by the left arrow corresponds to the {111}Σ3 GB while the one indicated by the right arrow to the {2$\bar{1}$1}Σ3 GB. The energy arising from the Wulff–Herring reconstruction is indicated by the dashed-black (solid-red) line if the points denoted by the left and right arrows (the four arrows) are used.*

GBs to faceting: The interface energy is reduced by the formation of low energy facets. The energy gain is large enough to compensate the increase in the total grain boundary area. The calculated grain boundary energies are a key input quantity for various mesoscale simulations. For example, these data will be used within the VIVIMAT project to study grain evolution [13,14] as relevant e.g. to understand and simulate the relation between microstructure, thermomechanical treatment and mechanical properties.

Comparing our results to previous theoretical data for the <110> tilt GBs in Al which were based solely on MEAM potentials and cluster calculations [15], our approach provides the advantage of projecting the accuracy of the small scale *ab-initio* calculations to the larger scale MEAM potentials calculations. Furthermore, in the present study, the construction of the atomic geometries of the GBs is based solely on symmetry operations within the framework of the CSL. The use of periodic boundary conditions restricts the interface planes to have the area and the misorientation defined by the aforementioned symmetry operations. This is the necessary first step in order to gather a more physical and mathematical formulation for the whole 5D space of the solid-solid interfaces. Indeed the calculated GBs may be in principle correlated to dislocation distributions and dislocation interactions. While for low angle GBs the misorientation angle is correlated to distribution of lattice dislocations, for high angle GBs the misorientation angles can in principle be treated as small departures from certain low Σ GBs. In the latter case the departure angles from the low Σ GBs can be correlated to distributions of secondary dislocations [16]. The correlation of the secondary dislocation distributions and interactions will be a natural next step of this work.

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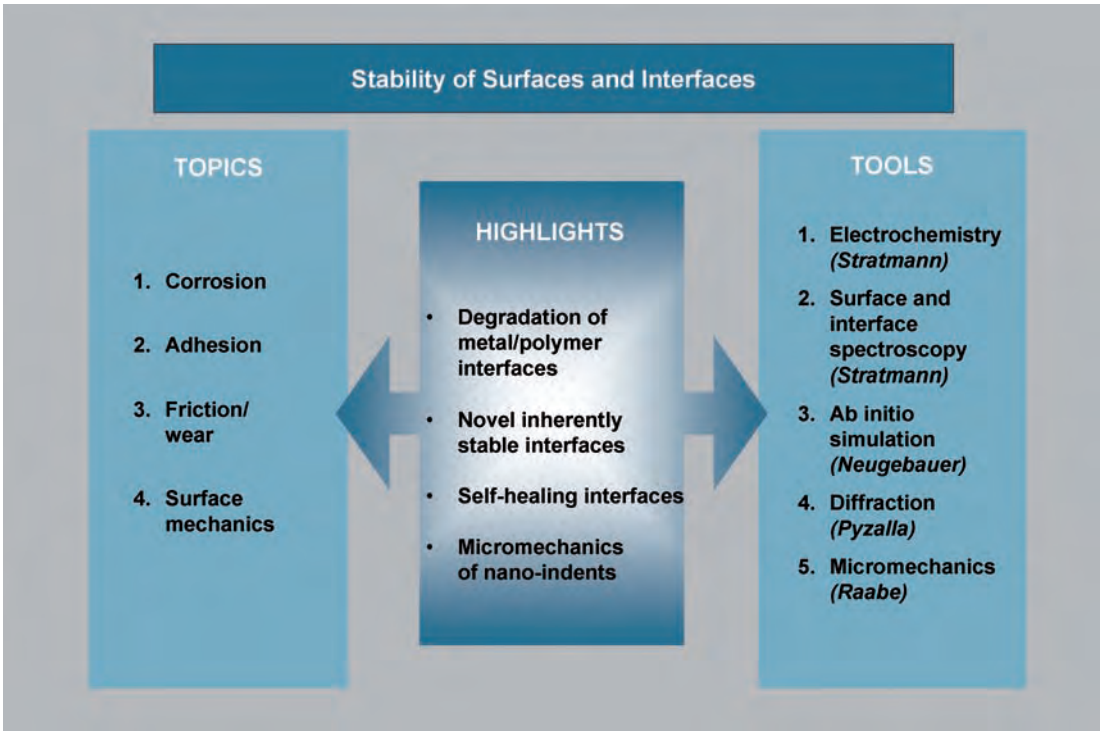
Stability of Surfaces and Interfaces

Introduction

Surfaces and interfaces are of crucial and ever increasing importance for material science. This is true even for bulk materials due to the continuously decreasing size of the main components of any material like grains or inclusions but it is in particular true for composites, for bonds between similar or dissimilar materials and for the properties of the surface itself. For structural materials like steels which are of dominant importance for the MPI für Eisenforschung some aspects are of particular relevance (see figure):

- All structural materials are highly instable from a thermodynamic standpoint of view. Therefore all materials tend to degrade by corrosion reactions as reversal of materials production process. These reactions are mostly exclusively surface reactions and typically at low temperatures electrochemical or at high temperatures chemical in nature. Protecting surfaces against corrosion reactions is essential for any material and usually a task which is part of any materials development. Corrosion research always used to be of top importance for the MPI für Eisenforschung.
- Composite materials and structural bonds are characterised by chemical or physical bonds between the dissimilar partners. Therefore adhesion determines the stability of the whole composite and any degradation of the bond strength will limits the materials use. Adhesion research within the MPI für Eisenforschung has two major aspects: the adhesion of polymers on metallic or oxidic substrates (department of M. Stratmann) and welds between similar and dissimilar materials (department of A. Pyzalla).
- In many times the surface stability is limited by the mechanical interaction between the materials and its environment. Frequently the mechanical interaction overlaps with a chemical and / or electrochemical attack of the surface. All these aspects are being investigated: friction and wear within the department of Anke Pyzalla and tribocorrosion within the department of Martin Stratmann.
- Besides chemistry and electrochemistry the mechanical properties of surfaces and interfaces are of considerable importance



for their reactivity and stability. During high temperature corrosion reactions cycling temperature conditions prevail frequently and then due to the different expansion coefficient of the scale and the bulk materials and due to the resulting stress cracking is observed. The measurement of surface stress is well established within the departments of Anke Pyzalla and Dierk Raabe, the theoretical treatment of surface mechanics is established with Dierk Raabe's group.

The tools which are necessary to study the structure, the mechanical properties and the reactivity of surfaces and interfaces are spread over all departments of the Max-Planck-Institut. The institute is unique in this respect.

The Department of Interface Chemistry and Surface Engineering (M. Stratmann) is specialised in the use of electrochemical techniques to detect the reaction rates and in the use of surface spectroscopy from UHV-type electron spectroscopy to optical spectroscopy to detect surfaces structures and surface chemistry down to atomic dimensions.

The Department of Computational Materials Design (J. Neugebauer) uses ab-initio type calculations to model surface reactions, surface structures and surface properties.

The Department of Microstructure Physics and Metal Forming (D. Raabe) is leading in mesoscopic simulation of surface mechanics.

The Department of Diagnostics and Technology of Steel (A. Pyzalla) uses diffraction and scattering techniques including synchrotron based radiation in the analysis of stresses and structures of surfaces and interfaces.

Some results of the institute's work in the area of surfaces and interfaces have recently drawn international attention. These are in particular:

- The physico-chemical analysis of degradation reactions at polymer/metal interfaces
- The detection of inherently stable metal/polymer interfaces based on semiconducting oxides
- The invention of self healing interfaces
- The detailed understanding of the mechanical properties of nano-indents
- Welding of dissimilar joints.

Some of these highlights are summarised in selected short papers in the following part of the scientific report.

As the MPI für Eisenforschung is unique in its combination of surface physics, electrochemistry, theory of surfaces and analysis of surfaces by a variety of techniques it is expected, that after the establishment of the new departments of Jörg Neugebauer and Anke Pyzalla the science of surface and interface degradation is further strengthened. This will include in future also aspects like hydrogen embrittlement in metals which is a property of the bulk material but is determined by the evolution of hydrogen as part of the electrochemical corrosion reaction. It is also easy to foresee, that the use of in-situ synchrotron based techniques will provide considerable new insight into corrosion reactions like the high temperature corrosion of high alloyed steels and Ni-based alloys.

Conducting Polymers for Corrosion Protection: Development of Intelligent Self-Healing Coatings and Probing the Hidden Mechanisms of Delamination

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Department of Interface Chemistry and Surface Engineering

Organic coatings are an efficient way to protect metal based products from corrosion. However, at the long-term scale even in the absence of defects in the coating a sufficient amount of ions may penetrate through the coating so that corrosion at the interface may occur. More dangerous are defects in the coating. Such defects may be caused by external attack, such as through impact by stones or scratches, or by production steps. For instance, forming of pre-coated steel sheet becomes of increasing importance in various fields of industrial application. However, forming of plastic material unavoidably results in at least nanoscopic defects at the interface [1], which have a direct negative impact on the coating performance.

In any case, sooner or later corrosion will occur at defects and cause electrochemically driven delamination of the coating. Especially the so-called cathodic delamination can be extremely fast (see e.g. [2]). Hence, in order to limit corrosive attack, corrosion inhibiting pigments are added to the paints.

The most efficient pigments are those containing chromates, but because of their toxic and carcinogenic nature their use has to be progressively decreased. In fact, nearly all powerful inhibitors may have detrimental effects on environment when released in substantial amounts. Since in basically all pigments the release of inhibitors is based on leaching, inhibitors are constantly released into the environment, even when they are not needed, thus presenting a permanent environmental problem. Hence, novel approaches are desperately sought for.

The first reports on a possible potential of intrinsically conducting polymers (ICP) for corrosion protection of metals were presented by Mengoli [3] and DeBerry [4], who studied the behaviour of polyaniline (PANI) electrodeposited on steel. Since then a large number of studies has been performed. As basically all studies focus on redox active conducting polymers, such as polyaniline, polypyrrole or polythiophene , in the following ICP refers to redox active polymers only. A number of different mechanisms are proposed, such as the so-called “ennobling mechanism”, that is based on the assumption that conductive redox polymers such as polyaniline or polypyrrole, applied in their oxidized state, may act as an oxidizer, improving the oxide layer at the polymer/metal interface (see e.g. [5]) or even maintain the metal in small defects in the passive domain [6,7]. A detailed analysis of the most postulated mechanisms was carried out at MPIE and it was shown that none of these can provide protection under general corrosion conditions [8].

However, an extensive overview over the overall research on conducting polymers for corrosion protection by ICPs by Tallman et al. and Spinks et al. [9,10], clearly shows that coatings containing ICPs can provide corrosion protection at least under some conditions. But the investigations at MPIE also clearly show that coatings performing well under immersion conditions and in the absence of larger defects are often observed to fail in the presence of large defects and under atmospheric corrosion conditions [11,8]. On the other hand, for some coatings based on conducting polymers even in the presence of larger defects good corrosion protection is observed [12-14].

The reason why good corrosion protection is often observed for immersed condition and in the absence of large defect while disastrous break-down occurs in the presence of larger ones has to do with how fast ICP reduction starting from the defect site will progress into the intact coating. Obviously, in a good coating the ICP in the vicinity of the defect (i.e. in galvanic contact with the defect, which is a larger amount of ICP in the case of immersion) can be activated and stop corrosion [8], i.e. by its reduction it can provide high enough oxidation power for passivation, but if the corrosion cannot be stopped this fast reduction results in a fast overall break down of the coating [8,11,14]. Hence, one important key factor for designing corrosion protection coatings based on ICPs is the understanding of what governs the reduction kinetics in the coating.

This will also be of importance for optimizing the one mechanism that seems to be the most powerful corrosion protection mechanism of ICPs: the intelligent release of corrosion inhibiting anions. Barisci et al. [15] for the first time pointed out that as a result of a galvanic coupling between the corroding metal and an ICP the polymer could be reduced and consequently dopants could be set free. If dopands with corrosion inhibiting properties are chosen, the release from the ICP might result in the inhibition

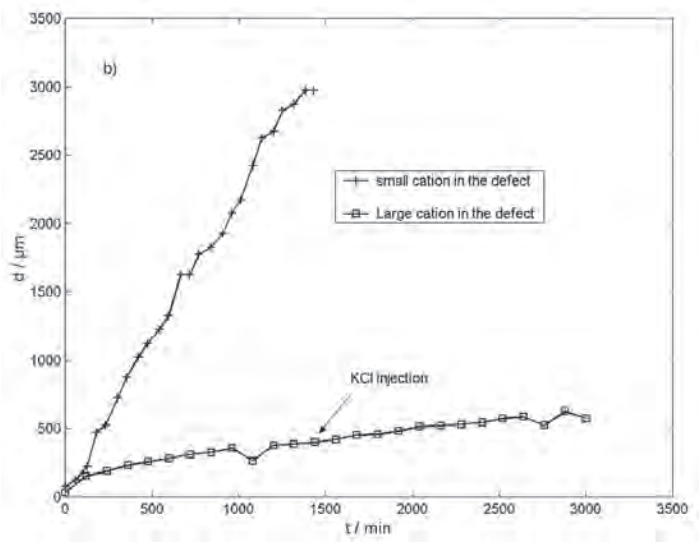

Fig. 1: *Comparison of the progress of the reduction front vs. time for chloride doped polypyrrole in the presence of a small cation in the defect (crosses) and for the case of the big tetrabutylammonium cation in the electrolyte (open squares, data). The injection of KCl has no effect on the slow curve started with only the big cation in the defect.*

of the corrosion in the defect or at least in a slow down of the coating delamination. Kinlen et al. [16] and Kendig et al. [17] showed that in the case of polyaniline anions can be released. Dopant release as a definitive consequence of electrochemical ICP reduction induced by decrease in potential, which always accompanies delamination originating at a defect, was found at MPIE by Paliwoda et al. [14].

Unlike for the case of standard corrosion pigments no leaching is observed in these cases, as the release of the anions is triggered by the corrosion activity at the defect. Especially the correlated interfacial potential change is an effective and very precise trigger for an intelligent release of corrosion inhibitors stored as dopants in the conducting polymer [14] ensuring a very case selective, really intelligent release for the case of polypyrrole, while for PANI most likely the correlated increase in pH will cause the release of the anions [16,17].

As reduction is linked to ion transport, because either anions have to be released or cations be incorporated, the electrochemical activity and of course the desired release of the anions will be linked to the electronic and especially the ionic conductivity of the polymer. It was the intention of this study to investigate the ionic conductivity of conducting polymers over length scales that are characteristic for realistic corrosion scenarios, i.e. over 100 microns or more. Usually, electrochemical studies on the release and incorporation properties of ions into conducting polymers are carried out on coatings of thicknesses in the range of a few microns.

For the studies performed at MPIE, a delamination set-up optimized for Scanning Kelvin Probe (SKP) investigation was chosen. The idea for this was triggered by our observation that for the case of atmospheric corrosion-like conditions, electrodeposited molybdate-doped polypyrrole coatings totally failed by fast delamination from a defect site (observed by SKP), not releasing the dopant at all [11,14], only incorporating cations, while for immersion and in presence of smaller defects dopant was released resulting in good corrosion performance [18]. The latter observation is in accordance with combined EIS and EQCM studies showing that these coatings show mixed anion release and cation incorporation during reduction [18].

In order to exclusively focus on the ICP reduction mechanism possible anodic side reactions had to be avoided. For this the polypyrrole coatings were prepared on inert gold substrates. The procedure was as follows: first the artificial defect was polarized to a negative potential similar to the corrosion potential of actively corroding iron while the atmosphere in the SKP chamber was oxygen free. This way only reduction of the ICP can occur. For the ICP reduction either anion release or cation incorporation, or a mixture of both, is necessary in order to ensure charge neutrality, so the contact between the polymer and the electrolyte at the defect is essential. Hence, the PPy reduction will proceed as a moving front from the border with the defect into the intact coating. This progress into the still un-reduced coating was monitored by SKP. The progress over time is shown in Fig. 1 for the case of polypyrrole doped with chloride. With KCl solution in the defect the reduction proceeds quite fast from the defect into the intact coating. When only tetrabutylammonium chloride, i.e. an electrolyte containing a large organic cation that cannot be incorporated into the polypyrrole, is in the defect the progress of the reduction front is much slower, even if later KCl is injected to the defect (see Fig. 1). In combination with additional

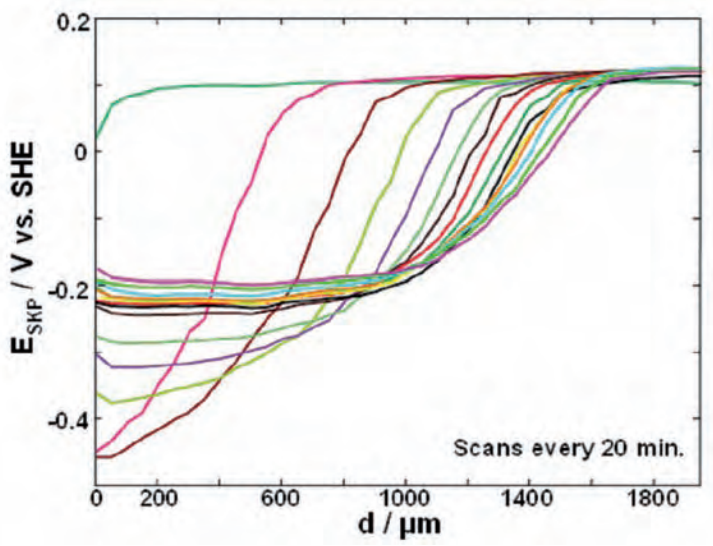

Fig. 2: *Potential profiles for the delamination of a composite coating containing polypyrrole nanoparticles doped with molybdate. After an initial phase the potentials in the delaminated area increase again, indicating passivation of the defect by released molybdate, and the delamination comes to a stop [14].*

electrochemical and analytical studies it could be shown that the fast reduction in presence of the small potassium cation is caused by fast cation mobility in the reduced polymer, which is due to the gradual transformation of the polymer into an "autobahn" for fast cation transport with increasing reduction progress. Even for ICPs which show for the case of standard immersion electrochemical reduction substantial anion release this mentioned transformation leads for the delamination case finally to an exclusive cation incorporation [19]. It was also shown that the coating delamination in air is governed by this polymer reduction, i.e. by the same cation transport. For fundamental reasons it is proposed that this is true for all kinds of redox polymer, regardless of kind of dopant, polymerisation conditions etc [19]. It is assumed that this fast cation transport will also occur in composite coatings of conducting polymer pigments or filaments in a non-conductive matrix polymer where high conductivity is reached by extended percolation networks of the conducting polymer. The cation transport would then occur via these percolation networks.

This is supported by the fact that reports on a supposed good corrosion performance of coatings based on continuous conducting redox polymers rely on immersion corrosion tests, while a convincing corrosion performance also under conditions similar to the atmospheric corrosion conditions with a defect in the coating simulated by the delamination set up of this study, seems only to exist for composite coatings (and indications are that indeed in these cases the percolation length is below or in the range of just one micron [14,19]).

Hence, for the design of corrosion protection coatings extended percolation networks of ICP have to be avoided. In Fig. 2 an example for a model composite coating is given, based on a composite coating containing polypyrrole nanoparticles (70 nm diameter, no extended lateral percolation network) doped with molybdate. As can be seen, after a while the potential in the already delaminated area increases as the inhibitor is released and passivates the defect, which causes the delamination to stop.

Recently, we also discovered that, also without inhibitor anions, a discontinuous ICP coating can provide superior protection against delamination. As an example, in Fig. 3 the delamination inhibiting performance of a pattern of individual PANI dots at the interface metal/coating is shown. It was observed that a delamination front approaching a "pocket" of buried ICP will be stopped in front of the ICP. The reasons for this are not fully known yet. At first it was assumed that the ICP might polarize the interface in its surrounding to such anodic potentials that no oxygen reduction can occur, the key reaction during cathodic delamination. However, the experimental results obtained so far indicate that this may not be the key factor. It is assumed that our current research on this topic will also provide novel fundamental insight into the mechanisms of cathodic delamination.

Summarizing, our results show that extended percolation networks of ICP are to be avoided. Only then the release of the inhibitor anion is guaranteed to take place even in presence of large defects at atmospheric corrosion conditions. Hence, not high conductivity, which requires extended percolation networks, is important for good corrosion protection, but electrochemical activity of a high amount of conducting polymer without allowing extended percolation networks. Now the problem is that for electrochemical activity the particles need to be in electric contact with the metal surface, either directly or by contact with other particles that are in contact

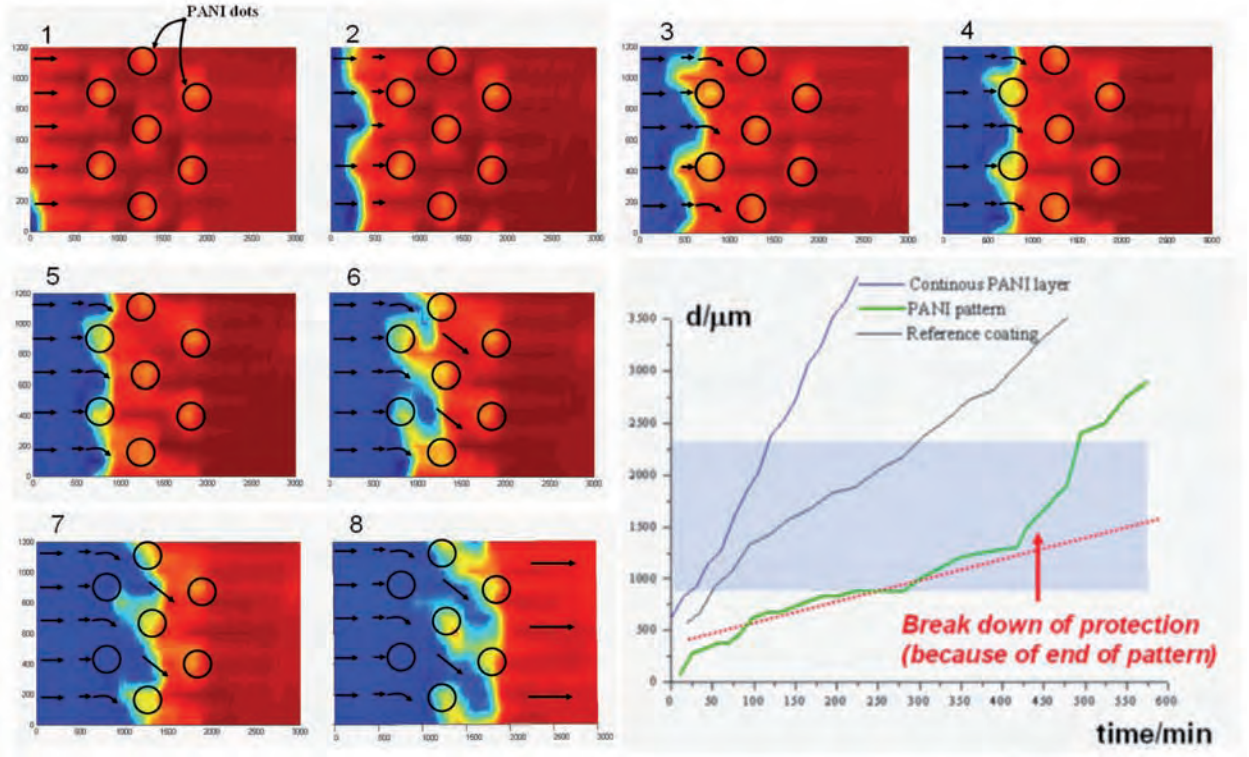

Fig. 3: *Progress of delamination through a pattern of PANI dots (time interval between scans is about 60 min). As can be seen in front of the pattern the delamination comes to a stop. Note how the delamination tries to avoid the patterns. As a result a delamination velocity about three times slower than without the PANI is achieved. Pure PANI would even be faster than the non-conductive matrix.*

with the metal surface, i.e. by percolation paths. For a composite coating without extended percolation networks this would result in most particles in the bulk of the coating being inactive, i.e. useless. Concluding, an optimisation between the prevention of macroscopically extended percolation networks and ensuring enough particles in the coating to be effective needs to be realised. Then very powerful novel corrosion protection coatings may be developed, based on a highly effective intelligent, case sensitive inhibitor release [14]. This is another subject of our current research.

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Probing the Adhesion Properties of Aluminum Oxy-Hydroxide Surfaces by means of Chemical Force Microscopy

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Department of Interface Chemistry and Surface Engineering

Understanding the effect of the pH on interactions of functional groups with surfaces is of fundamental interest for the understanding of phenomena like adhesion, de-adhesion and friction of organic coatings on an atomistic level. Modeling of the adhesive properties on a nanometer scale can be realized easily by preparing cantilever surfaces with different terminal groups by utilizing self-assembled monolayers on gold-coated AFM cantilevers. These model surfaces can be applied straightforward to measure the adhesion of these functional groups under varying conditions on various surfaces. This so-called chemical force microscopy [1] is therefore perfectly suitable for investigating the effect of the pH on the adhesion properties of functionalities like phosphonic or carboxylic acids, which are important adhesion promoters in corrosion resistant organic coatings and thin films. For a detailed understanding of the adhesion properties of organic coatings on aluminum oxy-hydroxide surfaces on the atomistic level it is of crucial importance to understand the complex interplay of adhesion promoting acid functionalities and the surface functionalities as a function of the pH. Consequently, the main focus of this work was to identify the different contributions to the overall adhesive force of phosphonic and carboxylic functionalities at different pH levels by means of chemical force microscopy.

Changing of the pH values leads to de-/ protonation of the acid functionalities on the AFM tips according to their pK_a value. E.g. increasing the pH value leads to an increasing negative charge density on the tip surface, while the ability to form H-bonds decreases (see Fig. 1a/b). Furthermore, oxide surfaces, like the aluminum oxy-hydroxide surface, are pH dependent as well. In acidic solutions the aluminum surface is positively charged due to the protonation of the surface hydroxide functionalities ($Al - OH_2^+$). In alkaline solutions the aluminum surface becomes negatively charged due to the amphoteric behavior of the aluminum, i.e. the possibility to accept an additional OH^- from the solution. The point of zero charge (PZC), at which the overall surface charge is zero, is at pH 8.7. As a consequence at this pH, the long-range Coulomb interactions with the negatively charged tip surface switch from attractive to repulsive, which can be observed in the approach curves of the force spectroscopy.

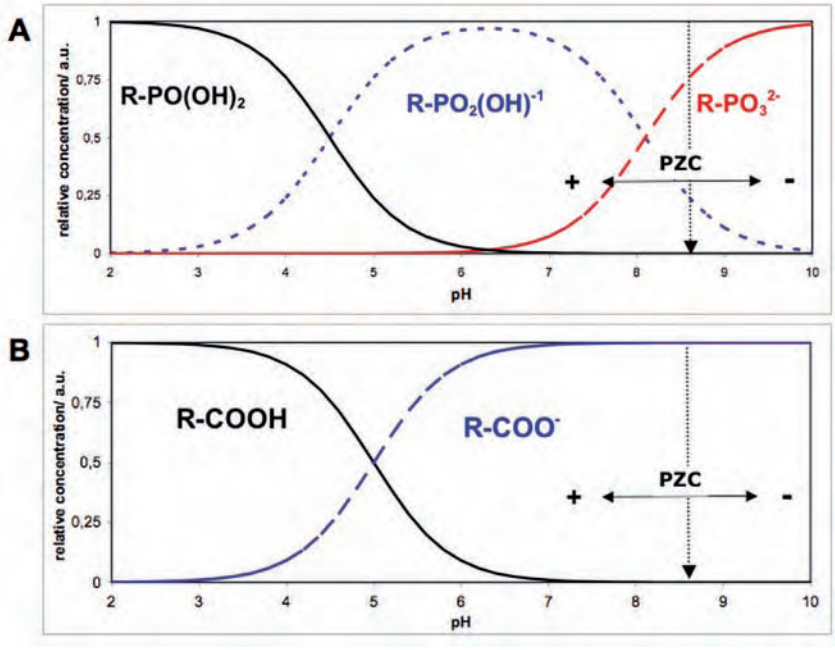

Fig. 1: *Schematic overview of the pH-dependent variations of the surface functionalities of (A) Carboxylic acid with pK≈5 and (B) Phosphonic acid with pK_1≈4.7 and pK_2≈8.4 terminated AFM-tip surfaces (for pK-values see [2]).*

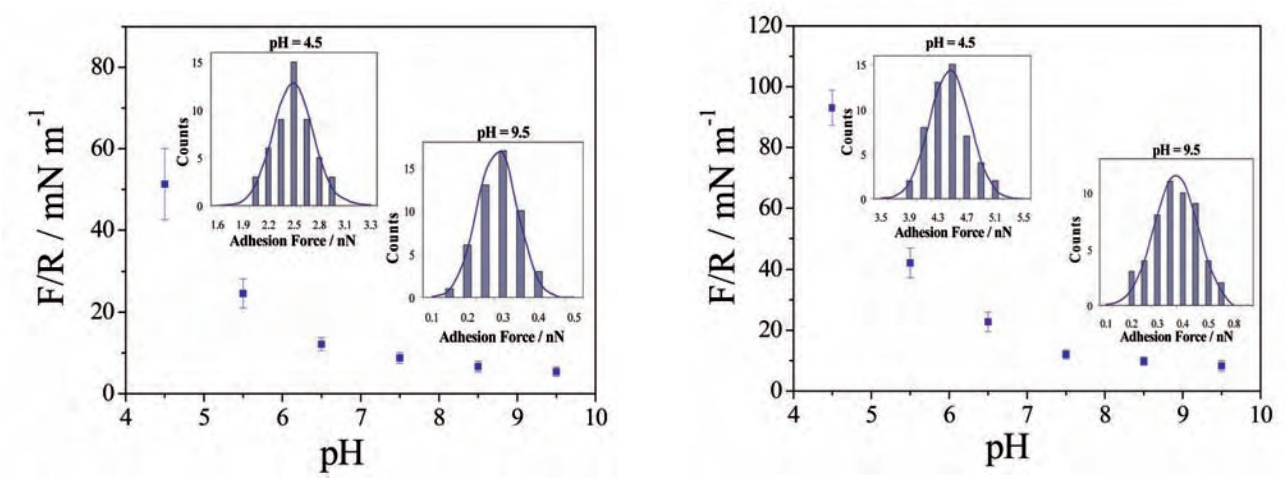

Fig. 2: *Adhesion force titration curve for tip modified (a) (12-Sulfanyldodecanyl-)phosphonic acid or (b) 11-Sulfanylundecanoic acid and aluminum substrate. Every pH-value represents an average of 50 curves.*

All chemical force measurements were performed on a JPK NanoWizard® AFM (JPK Instruments AG, Berlin, Germany) equipped with a custom-made liquid cell providing the possibility to change the electrolyte in situ. The measured adhesion force for the $-PO(OH)_2$ terminated tips decreased with increasing pH value as seen in Fig. 2a. Within the pH-range from 4.5 to 6.5 the phosphonic acid undergoes the first de-protonation step. According to literature [2], the out-of-plane OH groups of a phosphonic acid monolayer are considered to de-protonate in the first step, whereas the in-plane OH groups de-protonate in the second step. At pH 4.5 about half of the out-of-plane acid functionalities are de-protonated. Therefore, not only attractive Coulomb interactions between the positively charged aluminum oxy-hydroxide surfaces can contribute to the overall adhesive force, but H-bonds as well. Increasing the pH value leads to de-protonation of the out-of-plane OH-groups and therefore decreasing H-bonds normal to the surface (with the aluminum oxy-hydroxide surface) can be formed. The in-plane OH groups form H-bonds within the monolayer rather than with the aluminum oxy-hydroxide surface. At pH 6.5 the aluminum oxy-hydroxide surface still has a positive surface charge density, whereas the overall adhesive force decreases by more than 80%, even though the negative surface charge density on the tip increases significantly due to the almost entire de-protonation of the out-of-plane OH-group at this pH level. This reveals that the strong adhesion at lower pH values mainly results from H-bonds of out-of-plane OH groups or at least from their presence on the tip surface (a condensation reaction may be possible as well). Coulomb interactions are apparently not the crucial factor for the strong adhesion at lower pH values.

When shifting to higher pH values, such as pH > 8.7, the aluminum oxide surface becomes negatively charged as well, leading to repulsive Coulomb contributions to the overall adhesion force between the tip and the surface for measurements at pH 9.5. Accordingly, the adhesive force further decreases and the approach curves show a significant repulsive force at this pH value (see Fig. 3). This behaviour can be explained by the surface charge above and below the PZC of the oxide-covered aluminum surface. At a pH above the PZC repulsive Coulomb force, contributions between the now in sum negatively charged aluminum surface and the phosphonate group dominate the observed change of the adhesion force. There is no further detectable influence of the second de-protonation step but an increase of the surface charge density. This is not surprising because the in-plane OH-groups are not always considered to form H-bonds with the aluminum oxy-hydroxide surface.

The observed behavior of carboxylic acid terminated tips is qualitatively quite similar to the behavior of phosphonate terminated tips, whereby the adhesion force decreases with increasing pH value (Fig. 2b). At pH 4.5 a combination of protonated and de-protonated ($-CO_2^-$: $-CO_2H$ ≈ 1:3) groups can be expected. With increasing pH values the number of the carboxylate groups increases. The tip surface becomes increasingly negatively charged and loses the ability to form H-bonds. As observed for the phosphonate-terminated tip, the most significant decrease of the adhesion force occurred when increasing the pH from 4.5 to 6.5. Consequently, the strong adhesive force at lower pH values can be assigned to the formation of H-bonds, while more COOH groups become de-protonated, the adhesion forces decrease. Increasing of the pH to 9.5 yields fully dissociated surface functionalities on the tip and negatively charged aluminum oxy-hydroxide. As already discussed for the phosphonate terminated tip surface, the adhesion force further decreases as a consequence, and electrostatic repulsion was observed in the approach curves as well. This can

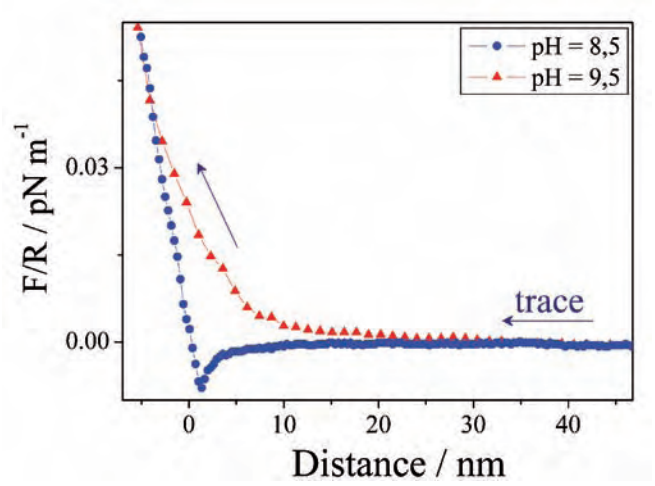

Fig. 3: *Approach curves at pH 8.5(blue symbols) and 9.5 (red symbols).*

be qualitatively argued in the same way as for the phosphonate-terminated tip surfaces before.

To conclude, the chemical force titration with these tips revealed that the strong adhesive forces at pH values below 6.5 are obviously a consequence of the increasing OH density on the modified tip surface that interacts with the aluminum oxy-hydroxide surface. Since the aluminum oxy-hydroxide surface is covered with OH functionalities mainly H-bonding interactions rather than electrostatic interactions contribute to the measured increase of the adhesion force at these pH values. The decrease of the adhesive force when shifting from pH 6.5 to pH 9.5 is attributed to the change of the electrostatic interactions from attractive to repulsive because changing the pH reverses the polarity of the aluminum oxy-hydroxide surface at the PZC. Nevertheless, it is obvious that the changes due to varying electrostatic interactions are small compared to the overall adhesive force within this pH range. Consequently, the adhesive force in this range seems to be mainly caused by van der Waals forces.

The investigations show clearly that the approach presented here enables the identification of the different contributions to the overall adhesive force of functional groups on oxide surfaces as a function of the pH. A tool could thereby be established which provides important insights into the chemistry of adhesion on a molecular level [3]. Anyway, there is still much work to be done in order to understand the complex interplay in more detail. Especially, an exact quantification of the different contributions in accordance with state-of-the-art theoretical models will be a crucial point for further investigations.

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Aluminium-Rich Fe_xAl_y Phases in Steel/Al Joints

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The necessity for lightweight constructions in automotive and other transportation industry has produced a strong interest in the joining of steels to Al-alloys. Today, most steel/Al-alloy joints are either form-fit or force-fit joints, which is due to the difficulties in substance-to-substance bonding arising mainly from the differences in the melting points of steel and Al-alloys, the differences in their thermal conductivity, the extremely low solubility of Fe in Al and due to the formation of intermetallic Fe_xAl_y-phases [1] as a consequence of chemical reactions and interdiffusion between Fe and Al.

As a consequence of the large difference in the melting points between steels and Al-alloys, the Al-alloy usually melts, while the steel remains in solid state in case of fusion welding. Thus, joining of Al-alloy to steel is usually achieved via filler, where the Al-alloy is welded to the filler material, while brazing occurs between the filler and the steel (Fig. 1).

We used a new metal inert gas welding technique, the so-called Cold Metal Transfer (CMT), developed at Fronius International GmbH for producing welds with lower heat input. The main characteristic that distinguishes the CMT welding process from conventional metal inert gas welding is the incorporation of the wire motion into process-control [2]. We aim at characterising the microstructure of the joints and in particular at identifying the intermetallic phases that form between the filler and the steel sheet. Details about the mechanical properties of the welds, their residual stress state and their formability in subsequent manufacturing processes are given in [3,4].

The intermetallic phase seam (IMP) in the CMT steel/Al welds (DX56D+Z140, 1mm/A6061-T4, 1mm/Al99.8-filler) is about 2.5 µm thick on average (Fig. 2) and thus, substantially thinner than intermetallic Fe_xAl_y phase seams observed in case of pressure welded joints and hot dip aluminised steel.

Phases in the IMP. The interface between the intermetallic phase seam (IMP) and the steel is heavily serrated, while the interface between the intermetallic phase and the Al 99.8 filler is rather smooth. Two phases with distinct morphologies appear within the intermetallic phase seam: large trapezoidal shaped grains are present at the steel side of the IMP, while at the interface between the IMP and the Al99.8-filler elliptical grains predominate, whose long axes usually are approximately perpendicular to the interface. By using transmission electron microscopy the large trapezoidal grains were identified as η-phase, which is a Fe_2Al_5 orthorhombic phase [5], the elliptical grains consist of the θ-phase, which is a $FeAl_3$ monoclinic phase [6]. The $FeAl_3$ grains contain a high density of microtwin boundaries (Fig. 3). In Fe_2Al_5, long individual dislocations and glissile dislocation half-

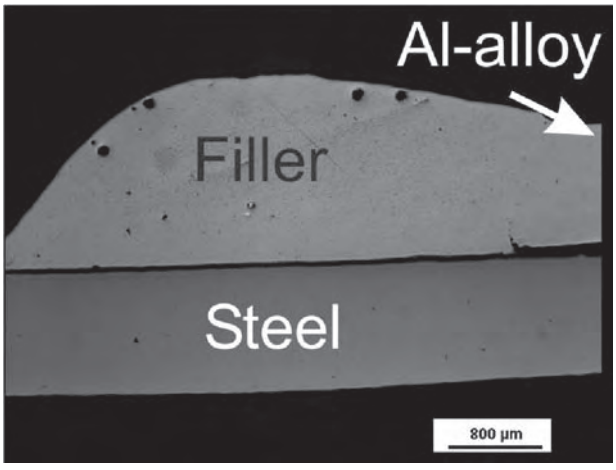

Fig. 1: *Macroscopic micrograph of the joint, where the Al99.8-filler welds with the Al-alloy plate and brazing occurs between filler and the steel plate.*

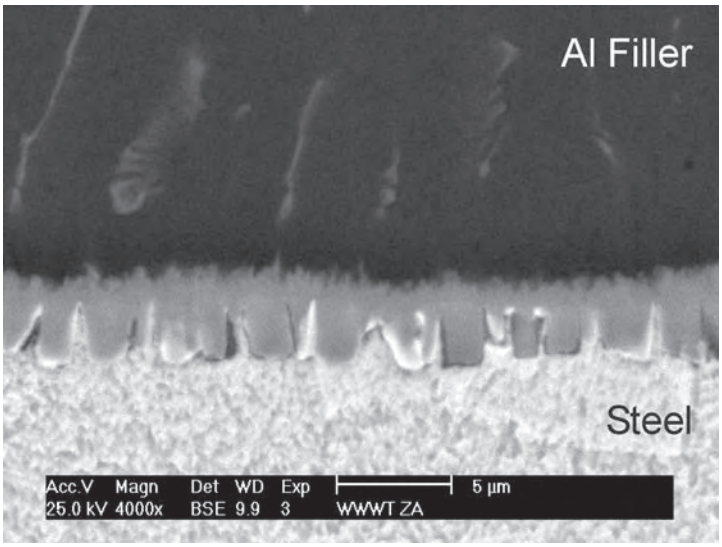

Fig. 2: *SEM-BSE micrograph of the intermetallic phase seam (IMP).*

loops can be observed (Fig. 4), which nucleate from the phase boundaries. They indicate that Frank-Read sources were activated at the straight part of the interface between Fe_2Al_5 and the $FeAl_3$. The finger-like areas in-between the Fe_2Al_5 grains belong to larger Al-enriched steel grains with up to 20% Al, which surround the individual Fe_2Al_5 grains. Near the interface to the Fe_2Al_5 a high dislocation density was observed in the steel grains.

Phase formation in the fusion welding process: The TEM investigations revealed that the long axis of the orthorhombic Fe_2Al_5 lattice is not perpendicular to the steel/Al-filler interface. Diffusion in the direction of the long axis of the orthorhombic Fe_2Al_5 lattice is known to be fastest, since this direction contains vacancies. In the IMP the volume fraction of Fe_2Al_5 is similar to that of $FeAl_3$. Both these observations indicate that chemical reaction beside interdiffusion plays a major part in the IMP growth.

The large size and the low number of the Fe_2Al_5 single crystals imply a very limited number of nuclei. Thus, contrary to e.g. [7,8], not the orientation of the longest axis of the Fe_2Al_5 but rather the nucleation conditions, as already suggested by [9], are the cause for the serrated structure of the steel-Fe_2Al_5 interface. The inclination of the longest axis of the Fe_2Al_5 to the direction perpendicular to the steel/Al 99.8 filler interface is probably due to a superposition of the directions of the temperature gradient perpendicular to the steel/Al 99.8 filler interface and the temperature gradient caused by the forward motion of the filler in the welding process.

The Fe_2Al_5 appears to be the phase formed first, since its interface towards the Fe_3Al is wavy, which indicates in a binary system, that it was a former interface between a liquid and a solid, while the straight interface of the Fe_2Al_5 on the steel side indicates solid-state diffusion [10]. This is in good

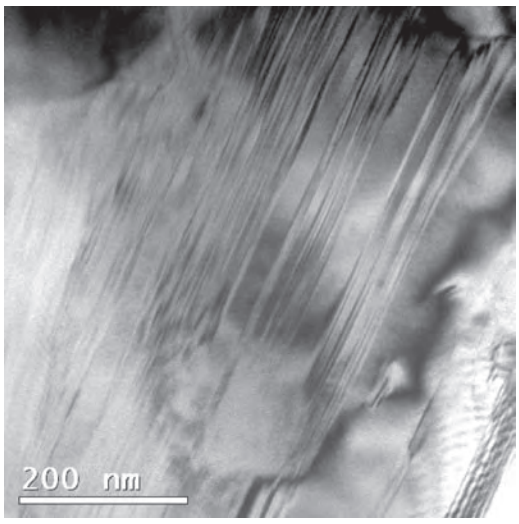

Fig. 3: *TEM-BF micrograph of microtwinning effect in $FeAl_3$.*

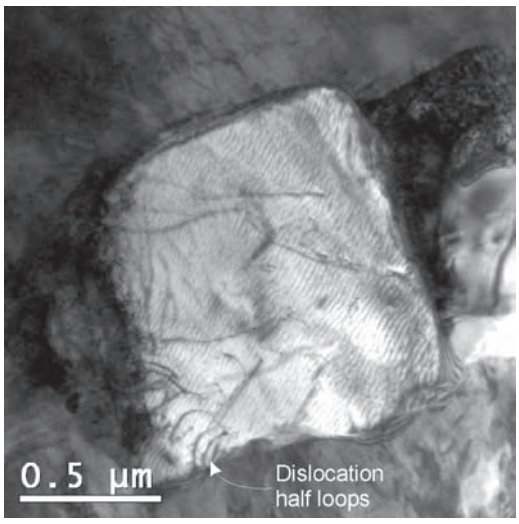

Fig. 4: *TEM-BF micrograph of a Fe_2Al_5 grain, showing glissile dislocation half loops as well as individual dislocations.*

agreement with [9], where $FeAl_3$ was formed during solidification of Al after withdrawal of the steel from the Al bath (in hot dipping tests). A further indication of the prior formation of the Fe_2Al_5 is the fact that each Fe_2Al_5 grain is a direct neighbour to several $FeAl_3$ grains, thus, it appears likely that the $FeAl_3$ nucleated at the interface of the already formed Fe_2Al_5.

The strong increase of volume during the formation of the $FeAl_3$ [11] results in high stresses, which may be responsible for the high microtwin density found in the $FeAl_3$ grains and for the dislocations in the Fe_2Al_5 grains. The low temperature of the weld pool and the cold surrounding material, that leads to rapid cooling, have prevented the disintegration of $FeAl_3$ in favour of Fe_2Al_5 and, thus, pore formation at the interface between $FeAl_3$ was not observed, although it occurred e.g. in diffusion couples [12] and TIG welds [13].

Further work will concentrate on systematic studies of the formation of aluminium-rich Fe_xAl_y intermetallics by chemical reaction and diffusion using diffusion couples, immersion tests and welding experiments. We aim at determining structure-property relationships for ternary Al-rich Fe_xAl_y intermetallics and subsequent optimizations of filler composition and properties of dissimilar steel/Al joints.

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Influence of Binder Composition and Nitridation on the Microstructure and Corrosion of (W,Ti,Ta,Nb)C-Co and (W,Ti,Ta,Nb)C-Ni Hardmetals

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Hardmetals, also known as cemented carbides, are composites consisting of hard carbide grains, usually WC, embedded in a tough and ductile metal binder. In order to improve hardness and wear resistance, other cubic carbides such as TiC, TaC, and NbC can be added to partially substitute WC. Hardmetals are used as cutting and drilling tools for ferrous and non-ferrous alloys, rocks, and wood. Wood cutting applications besides good wear resistance also require corrosion resistance of the hardmetals [1,2].

Because corrosion attacks preferentially the binder, the conventional Co-binder for hardmetals used in wood cutting applications in some cases has been substituted by Ni, which is intrinsically more oxidation resistant. Substituting Co by Ni, however, results in a decrease in wear resistance [3]. Another approach towards a higher corrosion resistance is the deposition of protective surface coatings to reduce the access of the aggressive medium to the bulk material. A drawback is that coatings are not applicable to many wear parts because of their geometry, dimension or because of extreme working conditions.

The alternative concept of increasing hardmetal corrosion resistance we followed is an increase in corrosion resistance by suitable tailoring of the microstructure by decreasing the amount of binder present in the surface of the hardmetal. Therefore, a nitridation treatment was applied to TiC-containing hardmetals [4,5]. The reaction between TiC and the sintering atmosphere e.g. N_2 or NH_3 leads to the formation of an outer-surface layer composed of (Ti,Ta,Nb)(C,N). The driving force for the formation of the carbonitride surface zone is the strong thermodynamic coupling between these refractory metals and N, which gives rise to inward N diffusion and outward Ti, Ta, and Nb diffusion. As an extra beneficial effect, the tool lifetime is increased since the Ti(C,N)-based hard phase is intrinsically more wear resistant than WC.

Here we present the main results obtained in the investigation of the influence of microstructure changes on the electrochemical behaviour of nitrided and non-nitrided (W,Ti)C-(Ta,Nb)C-Co/Ni hardmetals. A detailed study on the subject has recently been published elsewhere [6].

Microstructure before electrochemical tests. All samples show a uniform phase distribution in the bulk (Fig. 1). Prismatic WC grains (hexagonal crystal lattice) and spherical (Ti,Ta,Nb)C grains (also known as γ-phase, fcc crystal lattice) are embedded in the

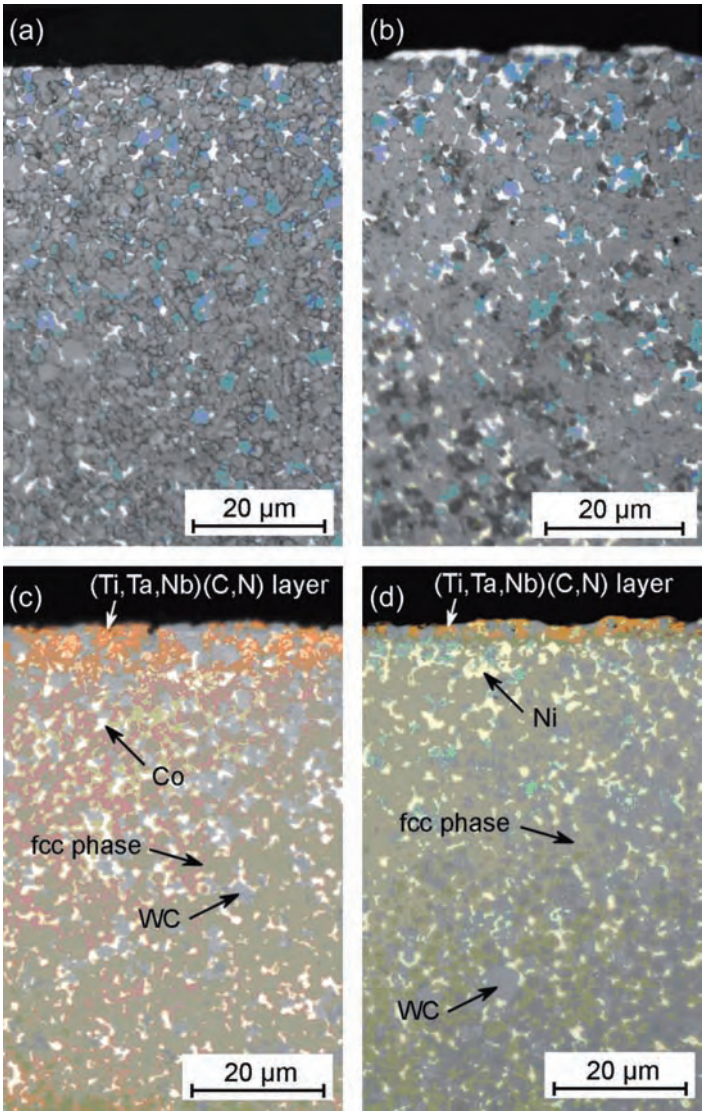

Fig.1: *Optical micrographs of non-nitrided (a) Co-binder and (b) Ni-binder. The effect of nitridation on the outer-surface microstructure in both hardmetals can be observed with (c) Co-binder and (d) Ni-binder.*

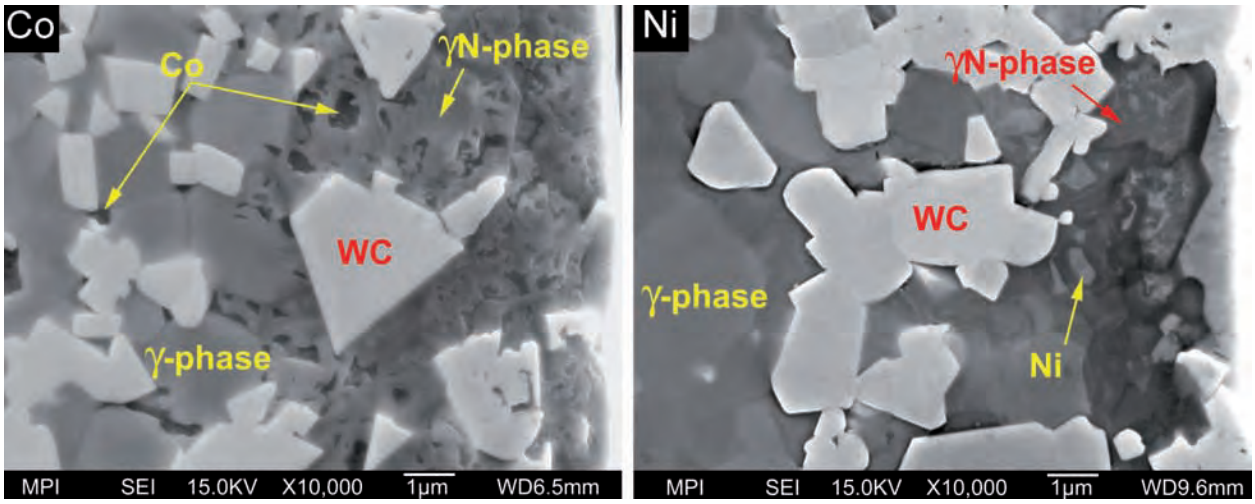

Fig.2: *SEM micrographs of cross-sections of nitrided hardmetals showing different morphologies of the γN-based outer-surface layer obtained according to the binder metal.*

metallic matrix. The binder system does not affect the binder mean free path and the average grain size of the hard phases in the bulk.

The nitridation treatment results in the formation of a (Ti,Ta,Nb)(C,N) solid solution (γN-phase) layer in the sample near surface area. This layer is twice thicker in the Co-base hardmetal compared to the Ni-base hardmetal. Also, the layer morphology is affected by the binder metal (Fig. 2). The average grain size of the γN-phase was determined as about 500 nm by synchrotron X-ray diffraction in grazing incidence. The fine grain size and change in morphology of the hard phases (from spherical to irregular shape) in the near-surface zone presumably leads to the improved plastic deformation resistance observed in the nitrided hardmetals.

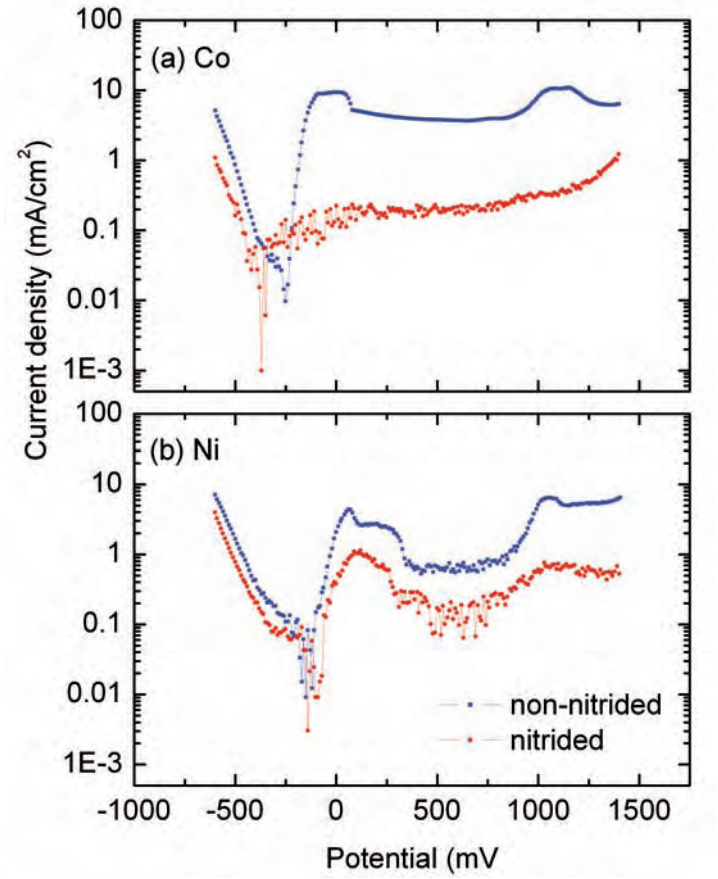

Fig.3: *Potentiodynamic polarization curves of non-nitrided and nitrided (a) Co-binder and (b) Ni-binder hardmetals.*

Electrochemical behavior. The corrosion resistance of the nitrided hardmetals was assessed by linear polarization electrochemical tests. We performed our tests at room temperature in 1N sulphuric acid solution open to air using a standard electrochemical cell. We chose to employ the linear sweep voltametry technique. Tests were carried out in two potential ranges to assess the oxidation behavior of distinct elements: (i) -600mV to +400mV and (ii) -600mV to +1400mV at a scan rate of 600mV/h.

The results of the corrosion tests (Fig. 3) reveal that an improvement of almost 4 times in corrosion resistance is achieved by the substitution of Co by Ni (see current densities). Corrosion resistance due to nitridation is increased by about 16 times in case of hardmetals with Co-binder and about 4 times in those based on a Ni-binder.

Corrosion of hardmetals in aggressive media mainly progresses by dissolution of the binder because of its lower redox potential in comparison to the carbides giving rise to galvanic coupling effects between these two phases [7,8]. The current densities determined in the electrochemical

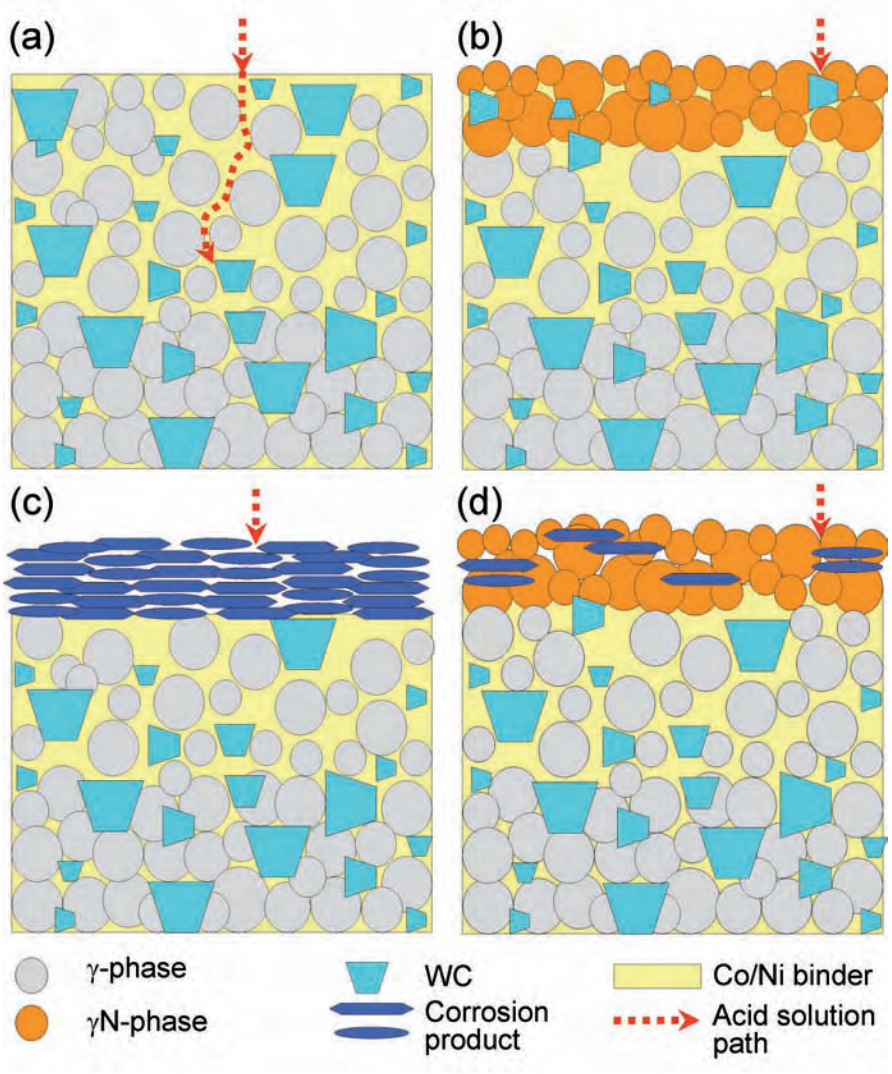

Fig.4: *Schematic of the structure of non-nitrided and nitrided hardmetals before (a) non-nitrided, (b) nitrided and after (c) non-nitrided, (d) nitrided binder dissolution, showing the effect of the surface morphology on the solvent access.*

measurements are related to the amount of binder consumed in the oxidation process and to the diffusion of metal ions into the electrolyte, which in its turn is determined by how easy or difficult the access of the corrosive medium to fresh binder is. We observe that this access strongly depends on the morphology of the binder inclusions.

Pseudopassivity. One of the explanations of this pseudopassivity is based on the increasing length of the Co diffusion path through the remaining porous hard phase skeleton left after dissolution of the binder. Since diffusion through this medium is slower (due to pore size and tortuosity of the structure) than free diffusion, the mass transport current flow should decrease [9]. We add to this argument the fact that the morphology and the type of porosity of the hard phase skeleton should be considered. A dense hard phase skeleton restricts the access of the solvent to the fresh binder in the bulk. The limiting case of such a dense hard phase skeleton is that of closed pores, where the solvent is almost completely denied access to the binder. Also, the decrease in the binder mean free path towards the bulk observed in the investigated hardmetals could account for the increasing difficulty for the corrosive medium to reach the inner binder (Fig. 4).

The results of our experiments show that the morphology of the phases in the near-surface zone plays a decisive role in inhibiting the corrosive attack. The main reason for the increase in corrosion resistance observed in the nitrided hardmetals is attributed to the formation of a binder-poor near surface zone. The closed porosity of the γN-based layer and the reduced binder mean free path at the surface strongly hinder the access of the acidic solution to the binder. Another aspect to be considered is the enhanced corrosion resistance of the γN-phase associated with the high chemical stability of the cubic refractory metal carbonitrides due to a strong degree of covalence in these materials.

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Scanning Tunneling Microscopy and Spectroscopy on Magnetic Surfaces: An ab initio Approach

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Introduction. Nanoscale magnetism is a topic of increasing interest, having potential applications e.g. in the development of ultra-fine grained materials or in advanced data storage materials. For the future development of this field it is essential to explore new materials having magnetic properties at or above room temperatures. One of the promising candidates are transition metal nitride systems since they can have magnetic properties ranging widely from ferromagnetic to antiferromagnetic, very high Curie and Néel temperatures, and very large magnetic moments. Recently, binary nitrides have been explored as model systems, with emphasis on the Mn_3N_2 (010) surface [1-5]. The surface magnetic properties were explored employing spin-polarized STM (SP-STM) that combines spin sensitivity with a well-known advantage of STM, namely, down-to single-atom spatial resolution. In contrast to conventional STM studies, SP-STM setup uses tips with a coating made of magnetic materials like Fe, Mn, or Cr. The tunneling current in SP-STM is then modulated by the angle between the spin of the tip and that of the sample — larger current for parallel orientation and smaller current for antiparallel orientation (Fig. 1(b)).

Although nowadays only a small fraction of STM experiments is devoted to study magnetic properties, the SP-STM has turned out to be a versatile and very successful tool to image both ferromagnetic and antiferromagnetic surface structures, magnetic nano-objects like magnetic clusters or chains deposited on different substrates to explore, e.g., competing magnetic interactions in clusters and between clusters and surfaces [6-7]. A crucial aspect to understand and interpret the experimentally obtained micrographs and to identify the underlying surface structure is the availability of accurate simulation tools to predict the micrographs for a given surface structure. The aim of the present study was to develop and test such an approach.

As a model case we consider the row-wise antiferromagnetic Mn_3N_2 (010) surface (Fig. 1(a)). As recently shown, the corresponding SP-STM image simultaneously contains both magnetic and chemical information [1]. Employing a method proposed by Yang and co-workers [1], the magnetic and nonmagnetic parts of the STM profiles can be separated (Fig. 2), and compared with the magnetic and chemical structure of the surface. Recently it was found that the magnetic STM image on Mn_3N_2 (010) depends strongly on the bias voltage, and that at a certain voltage the magnetic amplitude goes to zero and undergoes a contrast reversal (Fig. 3(a)-3(f)) [5]. Simultaneously the bias voltage dependence is also found to affect the SP-STM line profile shape. For this model system a straightforward interpretation of the detected STM profiles turned out to be not possible.

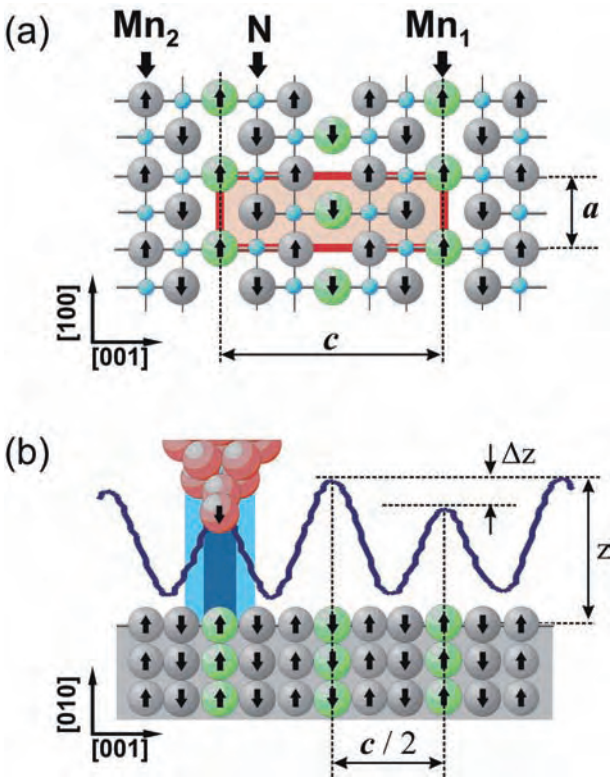

Fig. 1: *(a) Top view of the bulk terminated Mn_3N_2 (010) surface. Total magnetic moments are indicated as arrows inside the Mn atoms. The surface magnetic structure is row-wise anti-ferromagnetic along the [001] direction. Every third (001) plane of atoms lacks nitrogen, leading to the presence of differently-coordinated Mn_1 and Mn_2 atoms. (b) Geometrical configuration of the SP-STM experiment in the constant-current regime. The modulation of the tip-surface separation z is due to magnetic and nonmagnetic interactions between magnetically-polarized tip and anti-ferromagnetic surface. The measured peak modulation Δz is due to the magnetic interactions. The SP-STM profile is acquired at -0.1 V bias voltage employing an Fe-coated tip.*

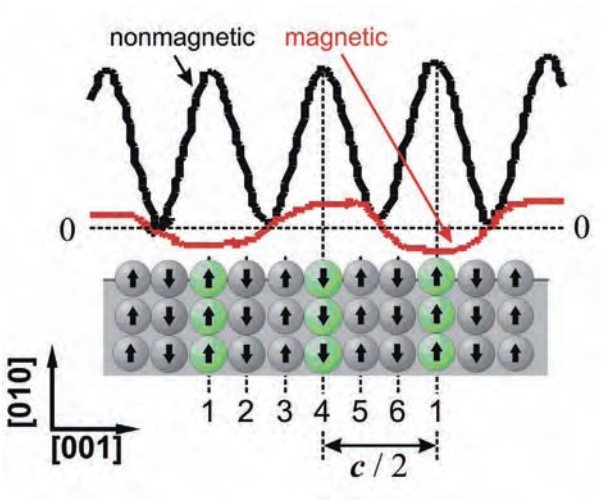

Fig. 2: *Nonmagnetic and magnetic components of the SP-STM image acquired at -0.1 V employing an Fe-coated tip. The rows of manganese atoms within the surface unit-cell are indicated by numbers 1 to 6.*

Theoretical Method. In order to understand the magnetic surface structure of $Mn_3N_2(010)$ on a firm theoretical basis, we have performed an ab-initio study. To elucidate the most thermodynamically stable magnetic and atomic surface configuration we have used a plane-wave norm-conserving pseudopotential approach as implemented in ABINIT [8]. The spin-PBE approximation was employed to describe exchange-correlation, since it is known to provide a more accurate description for transition metal compounds [5,9]. The bulk geometry has been calculated fully accounting for internal relaxations of the atomic structure. The surface has been modeled by a repeated slab geometry with a slab thickness of six atomic layers. The slabs have been separated by a vacuum region of 12 Å. Convergence checks showed the chosen slab and vacuum thickness to give error bars in the surface energy of less then 0.5 meV/Å^2.

To describe the SP-STM experiments, we have used the spin-polarized Tersoff-Hamann approach. Since the exact geometric, electronic, and magnetic properties of the tip used in the experiment are not known, and can even change during the experiment, the conventional approach is to assume that the electronic properties of the tip are independent of the applied bias voltage. The tunneling current then can be written as [1,5,10]:

$$I_t \sim \int dE\, [n^s(R_t, E) + P_t m^s(R_t, E)] \quad (1)$$

Here, the integration is performed over an energy window from the surface Fermi level E_{Fermi} to $E_{Fermi}+eV_{bias}$, $-1.0 \le P_t \le 1.0$ is the effective spin-polarization of the tip, $n^s(R_t,E) = \int dk \sum (\psi^{\uparrow}_{ik}(R_t)\,\delta(E-\varepsilon^{\uparrow}_{ik}) + \psi^{\downarrow}_{ik}(R_t)\,\delta(E-\varepsilon^{\downarrow}_{ik}))$ and $m^s(E) = \int dk \sum (\psi^{\uparrow}_{ik}(R_t)\,\delta(E-\varepsilon^{\uparrow}_{ik}) - \psi^{\downarrow}_{ik}(R_t)\,\delta(E-\varepsilon^{\downarrow}_{ik}))$ are nonmagnetic and magnetic local densities of states (LDOS) of the sample at the tip position R_t, respectively. $\psi^{\uparrow,\downarrow}_{ik}(r)$ and $\varepsilon^{\uparrow,\downarrow}_{ik}$ are the surface wave-functions and eigenvalues for quasiparticle states with band index i and k-vector k; arrows ↑ and ↓ refer to spin-up and spin-down channels accordingly.

It is well known that the typical tip-sample separation in conventional STM experiments remains between 5 and 15 Å. Due to exponential decay of the wave functions into the vacuum, however, a reliable description of the surface LDOS at tip-surface separations exceeding ~3 Å is hardly feasible within the plane-wave basis set. To overcome this deficiency, we have implemented a real-space approach to describe the vacuum region [11]. This approch provides an exact description of the

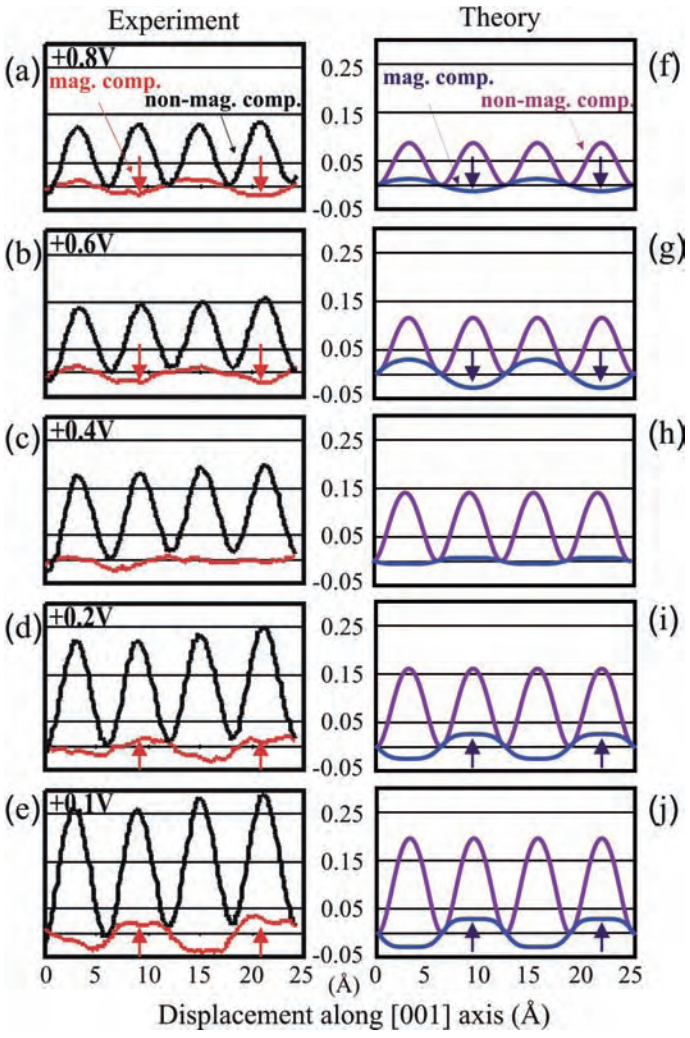

Fig. 3: *Magnetic and nonmagnetic height profiles for positive bias voltages. (a)-(e) Experimental nonmagnetic and magnetic profiles. (f)-(j) Corresponding theoretical nonmagnetic and magnetic height profiles calculated using spin-polarized DFT assuming tip with constant DOS.*

surface LDOS at any tip-surface separation. All STM simulations have been performed with a bias-independent constant tunneling current $I_t(V_{bias}) = I_{const}$, to model the experimental employed constant current regime.

Results and discussion. The results and a comparison with experiment are shown in Fig. 3. Figs. 3(f)–3(j) show the simulated nonmagnetic and magnetic SP-STM images obtained employing Eq.(1) for a tip with constant effective polarization P_t=15%. This value is similar to what has been assumed in previous theoretical studies [12,13]. The corresponding experimental profiles are shown in Fig. 3(a)-3(e). As can be seen, our theoretical ab initio approach provides an excellent agreement with experiment: It is clearly apparent that both simulated and experimental images show a magnetic contrast at all bias voltages and that a contrast reversal occurs at V_{bias} near +0.4 V. Moreover, at positive bias voltages the overall corrugation of the simulated profiles is largest at small bias magnitudes, whereas it is smaller at larger bias magnitudes, in agreement with experiment. Comparing the shape of the nonmagnetic profiles with the experimental ones, we find that both agree well showing a simple sinusoidal-like form. It is striking, that even small details of the simulated magnetic profiles are in remarkable agreement with experiment over the whole range of biases between -0.8 and +0.8 V; even the shape of the simulated and measured magnetic profiles coincides, being trapezoidal below +0.4 V and more rounded above this value.

Since the simulated profiles correspond to an electronically featureless tip, i.e., depend only on the surface electronic properties, we conclude that the experimentally observed magnetic contrast reversal can be adequately described solely in terms of the surface electronic structure. In Fig. 4, the contour plots of the surface spin LDOS corresponding to different applied bias voltages are shown. Only positive voltages relevant to the magnetic contrast reversal are presented. To elucidate the origin of the magnetic contrast reversal, we have projected the surface electron wave functions onto localized atomic orbitals. We have found that the spin-density contribution stemming from the Mn_1 atoms is mainly of the minority (with respect to the total magnetic moment of the corresponding atom) d_{xz} character, and remains essentially unchanged at all relevant positive biases. The Mn_1 atoms, therefore, cannot be responsible for the magnetic contrast reversal.

On the other hand, there is an evident bias dependency of the Mn_2 electronic properties. At small positive bias voltages, these atoms have predominant majority d_{z^2} character. These d_{z^2} orbitals are clearly distinguishable, e.g., in Fig. 4 as intense lobes

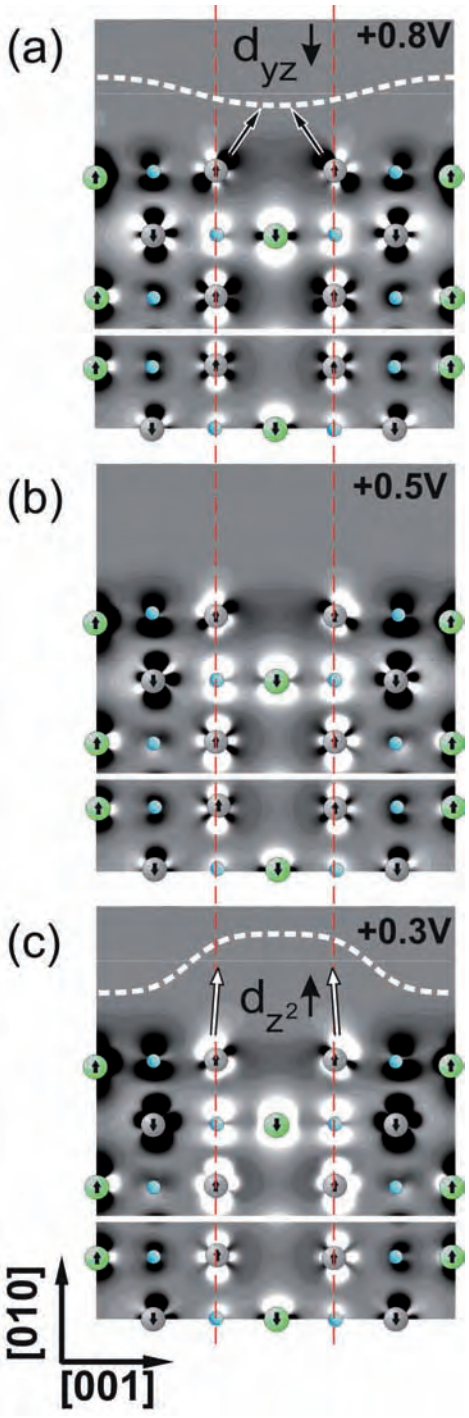

Fig. 4: *Evolution of the calculated surface spin-density with change of the bias voltage. Cross sections in the (100) plane calculated for slab (upper figures) and bulk (lower figures) and corresponding to bias voltage +0.8 V (a), +0.5 V (b), and +0.3 V (c) are shown. Arrows inside Mn_1 and Mn_2 atoms indicate their total magnetic moments; nitrogen atoms are shown as small balls. Bright and dark regions correspond to spin-up and spin-down densities correspondingly. Vertical dashed lines indicate rows of Mn_2 atoms that effectively screen contribution of Mn_1 atoms located in-between. The schematic contribution of the majority d_{z^2} orbitals leading to the trapezoidal shape of the magnetic height profile (+0.3 V) and contrast-inversed sinusoid-like profile (+0.8 V) due to the minority d_{yz} orbitals are shown as white dashed curves.*

located on top of the Mn_2 atoms. Since the Mn_2-Mn_1-Mn_2 rows of surface atoms are row-wise aFM, the minority contribution of Mn_1 atoms is of the same sign as the majority contributions of the surrounding Mn_2 atoms. The overlap of the minority d_{xz} lobes of Mn_1 atoms with the majority d_{z^2} lobes of the surrounding Mn_2 atoms results, therefore, in the total (↑↑↑↓↓↓) pattern at all distances above the surface. As the bias voltage V_{bias} increases, the spin character of Mn_2 atoms evolves smoothly from the majority d_{z^2} to minority d_{yz}. This can be seen in Fig. 4 at +0.5 and +0.8 V, where the minority d_{yz} orbital lobes become more prominent. These lobes tend to overlap on top of the neighboring Mn_1 row above the hollow site positions. At sufficiently large bias voltages, the minority d_{yz} of the Mn_2 atoms effectively screens the minority d_{xz} of the Mn_1 atoms and becomes dominating in the surface spin LDOS. This leads to the inverse of the magnetic pattern, e.g., from (↑↑↑) to (↓↓↓) and vice versa. At sufficiently large positive biases the effective (↓↓↓)(↑↑↑) magnetic pattern corresponds to (Mn_2↑Mn_1↓Mn_2↑)(Mn_2↓Mn_1↑Mn_2↓) rows of manganese atom moments.

Conclusions. In summary, we have developed an ab initio based tool to theoretically predict and analyze bias-dependent micrographs obtained by SP-STM on surfaces exhibiting nanomagnetism. The applicability and predictive power of the approach have been demonstrated for a model system, the aFM Mn_3N_2(010) surface.The theoretical results have been found in excellent agreement with measured profiles and allowed an in-depth interpretation of all major effects such as the magnetic contrast reversal and even subtle details affecting the specific shape of the line profile could be explained.

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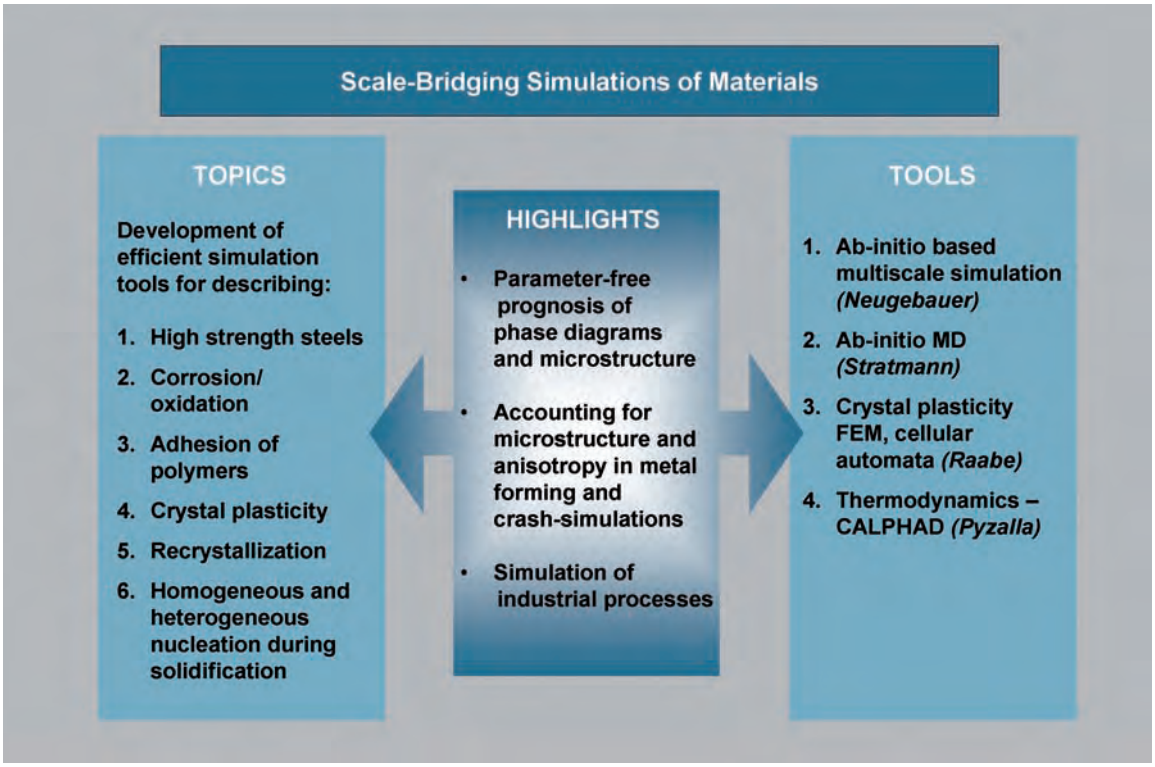
Scale-Bridging Simulations of Materials

Introduction

Another major field of activity and expertise of the institute is computational and experimental materials simulation. Due the inherent multiscale character of engineering materials, properties and processes, such as mechanical strength, plasticity, life time or corrosion resistance, can be traced back on various levels of the microstructure (multi grain structure, precipitates, dislocation mobility, etc.) and eventually on the atomic structure and the formation of chemical bonds.

In the last six years the institute has developed and applied state-of-the-art simulation tools to describe and predict materials properties with the main focus on the mesoscopic/macroscopic scale. Examples are the simulation of thermodynamic phase equilibria and diffusion in the group of Prof. Inden or the development of finite element (FEM) approaches which fully incorporate crystal plasticity and which go well beyond the capabilities of conventional FEM codes. The first case, the development and application of modeling tools to describe thermodynamics and diffusion of ternary alloys, is described in the following paper by Eleno et al. The second case, the use of the crystal plasticity approach is discussed in the papers of Zaafarani et al. and Bieler et al. The first one focuses on nanoindentation as is nowadays important to examine the materials response upon the application of localized loading. By performing a joint experimental study employing 3D-EBSD and employing crystal plasticity to model nanoindentation a detailed understanding of the deformation mechanisms could be achieved. The paper of Bieler et al. focuses on microcrack nucleation, a mechanism highly relevant to understand/prevent mechanical failure. Based on this study it became e.g. clear that the currently dominating paradigm for predicting damage nucleation – which assumes criteria based on a maximum stress or strain criterion – has to be replaced.

Recently, the institute has extended its simulation expertise also on the atomistic scale by opening in 2005 the Department of Computational Materials Design (Neugebauer). With the availability of the ab initio (i.e. fully parameter free) based multiscale simulation tools developed and applied in the CM department the institute is now able to apply two



complementary tools to describe materials: The top down approach as used e.g. in the Department of Microstructure Physics and Metal Forming (Raabe) where simulations start at the macroscale and are refined by mesoscale structural properties such as dislocation densities when needed. The other approach – the bottom-up approach – is followed by the CM department and the ab initio group by Dr. Blumenau in the Department of Interface Chemistry and Surface Engineering (Stratmann). The key idea here is to start on the most fundamental level describing materials properties, i.e., on the quantum-mechanical description of the electronic structure. The latter directly describes and determines the chemical bonds which in the end are the origin of all relevant materials properties. Therefore, this approach starts from a fully parameter free description on the atomistic scale. In combination with mesoscopic approaches such as thermodynamics, kinetics, or statistical mechanics it allows a parameter-free description also of mesoscale properties. A prerequisite to connect ab initio calculations with mesoscopic concepts is the availability of an efficient and flexible computer code. The paper by Boeck and Neugebauer gives a brief overview about some aspects of the methods and computer codes developed in the Department of Computational Materials Design.

Examples about the opportunities which the application of this approach opens are given in the papers by Blumenau et al. and by Grabowski et al. The first one describes how ab initio calculations in close collaboration with experiment allow to get a fundamental understanding of electron transfer reaction at polymer/metal interfaces. These reactions are important to e.g. understand and control polymer delamination at polymer/metal interfaces, a topic which is of great technological relevance since it promotes corrosion of the underlying metal. The second paper shows the great potential of combining ab initio tools with mesoscopic concepts such as thermodynamics. As described in this paper the approach allows to calculate fundamental thermodynamic properties such as heat capacity, thermal expansion, free energy solely on the computer, i.e., without the input of any experimental data. In the future this methodology will be combined with the well established CALPHAD approach to calculate phase diagrams.

Modelling Thermodynamics and Diffusion in bcc Fe-Rh-Ti

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The Fe-Rh-Ti system is characterized by a strong ordering tendency in the three binary sub-systems. A sound thermodynamic description of this system can only be obtained on the basis of a sophisticated treatment of the ordering reactions. In the present instance the Cluster Variation Method (CVM) in the Irregular Tetrahedron (IT) approximation has been chosen. In a previous study [1], prototype calculations were performed showing the various types of phase diagrams obtained as function of the choice of CVM interaction energies. However, there remained major discrepancies between calculation and experiments, which showed that more parameters are needed to obtain a satisfactory description of the system. It was the aim of this work to perform a new assessment of the Fe-Rh-Ti system to provide a good thermodynamic description which can be used for discussing the thermodynamic driving forces and diffusion paths in ternary diffusion couples. The complete calculations and experimental work has been submitted to Intermetallics [2, 3].

Two isothermal sections of the ternary system Fe-Rh-Ti were determined experimentally at 1000°C and 800°C using annealed alloys and diffusion couples [2]. No ternary compound was found in this system. The B2 ordered phase is stable in all three binary sub-systems of the Fe-Rh-Ti system and forms a continuous solid solution at both temperatures. Within the B2 phase domain, pseudo-interfaces were observed when the diffusion path crosses equi-atomic compositions. A large miscibility gap between A2 and B2 was observed in the Fe-rich part of the Fe-Rh-Ti system. The relevant ternary diffusion couple results are shown in Fig. 2 (next page), together with the CVM calculations.

The Cluster Variation Method (CVM) was proposed in 1951 by Kikuchi [4] in order to describe ordering phenomena. It was later applied to alloy phase diagram calculations [5, 6]. The method has been thoroughly described in the literature (see for example [7-10]). In the CVM approximation, the thermodynamic functions are written in terms of a maximum interaction range given by the basic cluster. In the present study the irregular tetrahedron (IT) in the body-centred cubic (bcc) parent lattice was chosen as basic cluster. With this choice, the long range ordered structures B2, B32 and $D0_3$, observed in the bcc lattice, can be described by the occupancy of the four sub-lattices [1, 10], defining the irregular tetrahedron shown in Fig. 1. It is customary

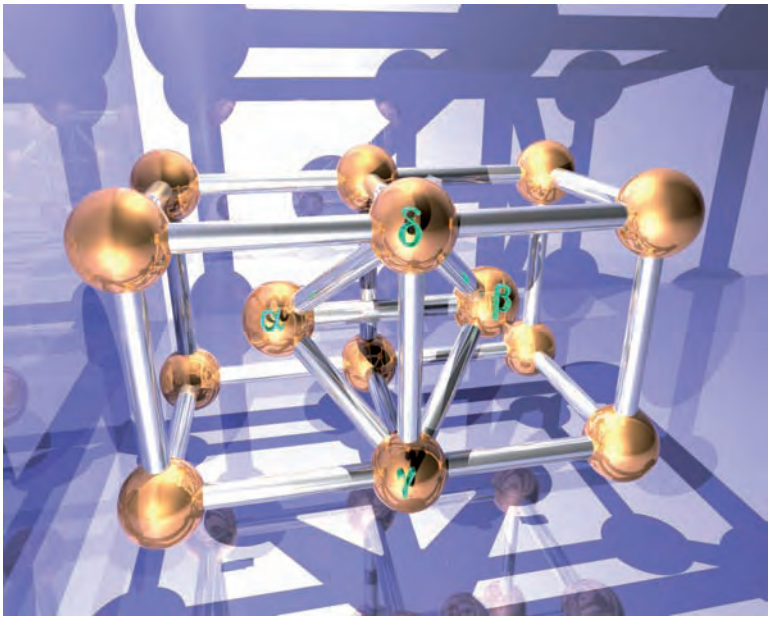

Fig. 1: *The Irregular Tetrahedron (IT) in the bcc lattice, the basic CVM cluster employed in the present work. The IT is defined by the four sublattices in the original crystal, indicated by* α, β, γ *and* δ.

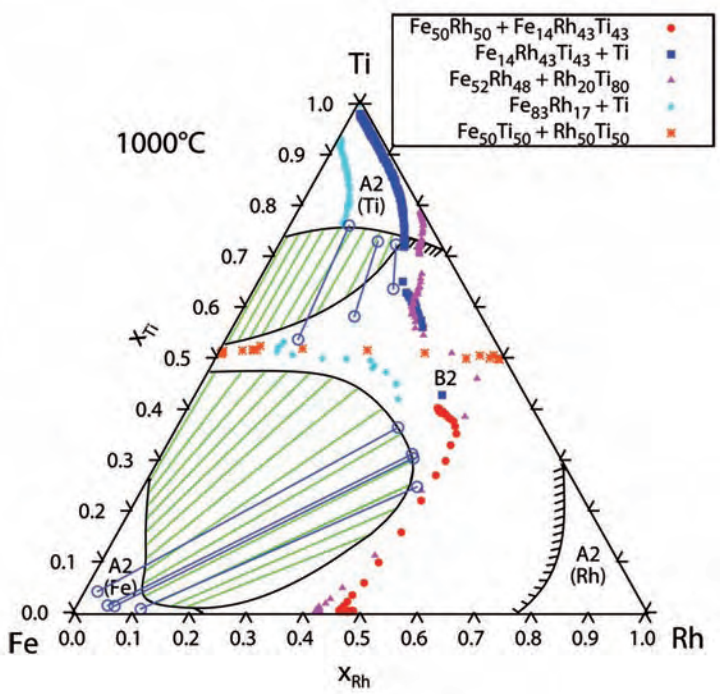

Fig. 2: *Comparison between the experimental data (blue tie-lines) and the CVM calculation in the bcc lattice. The diffusion paths shown (points) have end-members given in the textbox.*

to write the CVM energy parameters separating the contributions of pair interactions and multi-site interactions. The set of parameters used in this work is listed in Table 1, together with the formation energies of the bcc ordered structures at 0K.

In the binary Fe-Rh system the experimentally determined A2/B2 transition can be well reproduced assuming just a nearest neighbour pair interaction $\omega^{(1)}_{FeRh} = -800$ (k_B-units). The derivation of the CVM interaction parameters for the Fe-Ti binary system was described in a previous work [11]. Experimental tie-lines and enthalpies of formation were used as input for the determination of the parameters In the binary Rh-Ti. The A2/B2 transition was determined at 956°C and 1000°C [12].

The nearest-neighbour pair interaction parameter for the Rh-Ti system, $\omega^{(1)}_{RhTi} = -2100$ (k_B-units), was taken from Ref. 1, where it was deduced from the experimental enthalpy of formation of the stoichiometric B2 phase: $\Delta^0 H^F_{RhTi}$ = -71 kJ/mol [13]. The other parameters were introduced to improve the fit to the binary phase diagrams.

Table 1: *CVM interaction parameters used in the present calculations and formation energies at 0 K for the bcc structures possibly described in the CVM-IT approximation. Energies in units of the Boltzmann constant (1 k_B-unit = 8.31451 J/mol = 8.6174 ×10^{-2} meV/atom). The reference state is the mechanical mixture of the pure components, i.e., non-magnetic bcc Fe, Rh and Ti at the same temperature of the alloy.*

I - CVM interaction parameters						
Binary parameters					Ternary parameters	
A-B	$\omega^{(1)}_{AB}$	$\omega^{(2)}_{AB}$	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{ABAB}$	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{ABBB}$	$L2_1$-type	$F\bar{4}3m$-type
Fe-Rh	-800	0	0	0	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{FeFeRhTi} = 0$	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{FeRhFeTi} = 0$
Fe-Ti	-840	+650	-600	0	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{RhRhFeTi} = -300$	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{RhFeRhTi} = 0$
Rh-Ti	-2100	-300	-520	0	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{TiTiFeRh} = -50$	$\tilde{\omega}^{\alpha\beta\gamma\delta}_{TiFeTiRh} = -300$

II - Energies of formation at 0 K							
Binary structures					Ternary structures		
A-B	$D0_3$-A_3B	B2	B32	$D0_3$-AB_3	A_2BC	$L2_1$-type	$F\bar{4}3m$-type
Fe-Rh	-1600	-3200	-1600	-1600	Fe_2RhTi	-3730	-2765
Fe-Ti	-705	-3360	-3330	-705	Rh_2FeTi	-6625	-4189
Rh-Ti	-4650	-8400	-8220	-4650	Ti_2FeRh	-6180	-5015

Ternary interaction parameters were introduced in order to obtain a better reproduction of the experimental tie-lines in the ternary system near the Rh-Ti and Fe-Ti binary systems. Fig. 2 shows the agreement between the experimental results and the calculation, in an isotherm at 1000°C.

The bcc states in the Fe-Rh-Ti system exhibit strong ordering. Without appropriate model calculations, it is very difficult to get an idea of the driving forces for inter-diffusion and of their variation with composition. Their knowledge is mandatory for an understanding of the diffusion paths in the ternary diffusion couples. The Cluster Variation Method (CVM) in the tetrahedron approximation provides information about the variation of diffusion potentials.

The number fixed reference frame for solving the diffusion problem in a ternary system A-B-C is defined by $J_A + J_B + J_C = 0$, i.e., the flux of any selected component is opposite to the sum of the fluxes of the two other components, e.g. $J_C = -(J_A + J_B)$, since we are not taking vacancies into account. Diffusion in the ternary system is then described by a set of two equations [14]

$$J_A = -\frac{L_{AA}}{T}\nabla(\mu_A - \mu_C) - \frac{L_{AB}}{T}\nabla(\mu_B - \mu_C)$$
$$J_B = -\frac{L_{BA}}{T}\nabla(\mu_A - \mu_C) - \frac{L_{BB}}{T}\nabla(\mu_B - \mu_C) \qquad (1)$$

The definition of the reference frame also implies that the coefficients have to fulfil the relation

$$\sum_{J=A,B,C} L_{IJ} = 0 \qquad for\ I = A,B,C \qquad (2)$$

If one of the components diffuses much slower that the others, the diffusion of this element determines the diffusion path. Suppose B is this controlling element; then it follows from eq. 1 that the diffusion path follows a line $(\mu_A - \mu_B) = const.$ In this case the gradient $grad(\mu_A - \mu_C)$ vanishes and the flux of A is controlled by the diffusion of B. If A is the controlling element the path follows a line $(\mu_B - \mu_C) = const.$ In Fig. 3 the calculated isothermal section of the Fe-Rh-Ti phase diagram at T=1000°C is shown with lines of constant chemical potential differences $\mu_I - \mu_J$. In the triangular representation these lines originate from the corresponding binary sub-system I-J where they define the composition and they end at the vertex of the third component. The diagrams show regions of high density of lines indicating very strong variations with concentration. Along stoichiometric sections, $Fe_{0.5}Ti_{0.5}$- $Rh_{0.5}Ti_{0.5}$ and $Fe_{0.5}Rh_{0.5}$- $Rh_{0.5}Ti_{0.5}$, the iso-potential lines become very dense and almost parallel to these sections.

Fig. 4 (next page) shows the variation of the chemical potential differences within the section $Fe_{0.5}Ti_{0.5}$- $Rh_{0.5}Ti_{0.5}$, calculated by CVM using the parameters described above. Within the major part

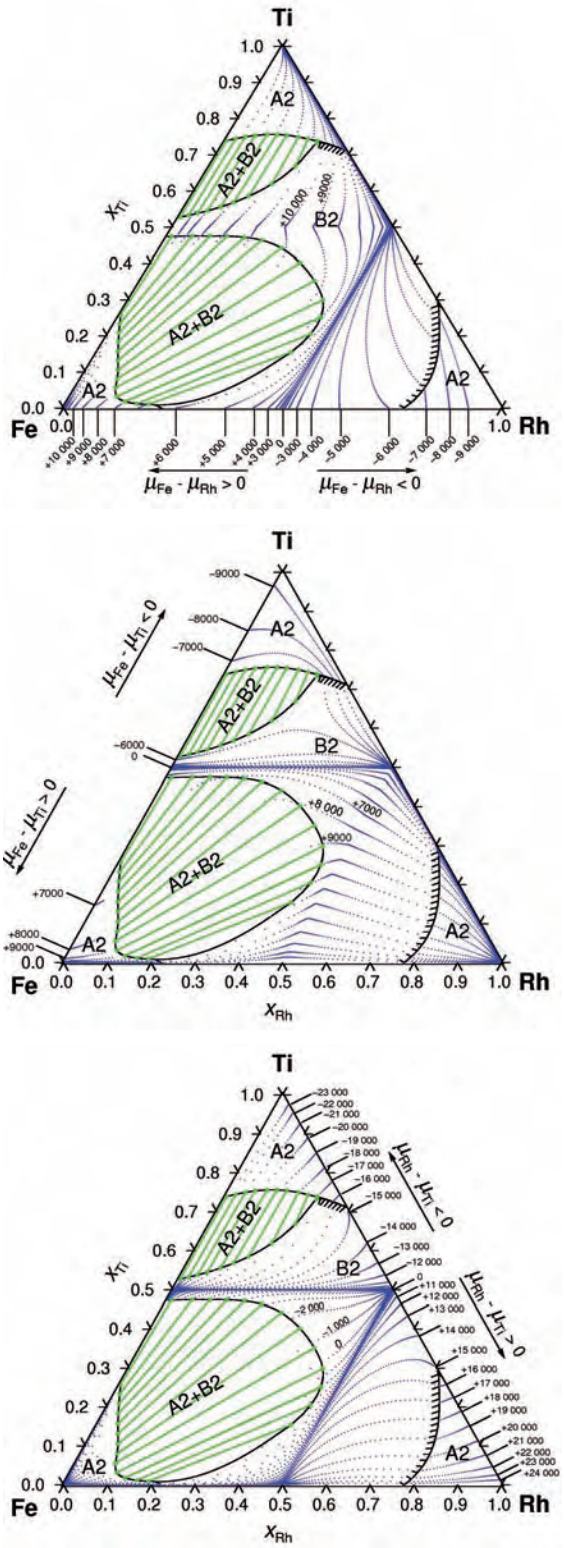

Fig. 3: *Iso-potential lines at 1000 °C (1273 K) calculated with the CVM in the IT approximation. Values are given in k_B-units. (a) $\mu_{Fe} - \mu_{Rh} = const.$ (b) $\mu_{Fe} - \mu_{Ti} = const.$ (c) $\mu_{Rh} - \mu_{Ti} = const.$*

of the composition range, $0.04 < x_{Rh} < 0.46$, the potential differences show a small variation with composition. Consequently, the required driving force for diffusion has to be made available by a steep gradient in composition. The opposite holds for the composition ranges close to the binary subsystems. The composition profile of the diffusion couple thus

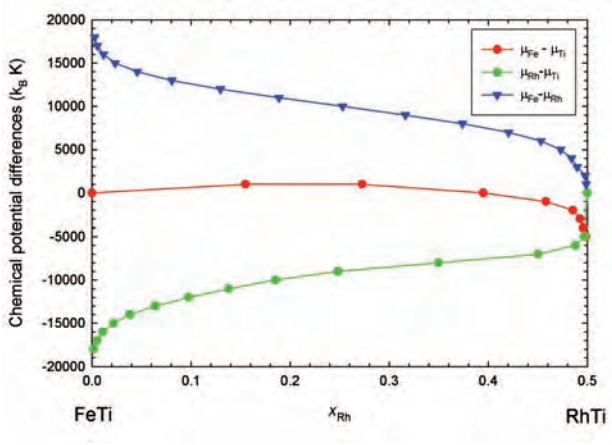

Fig. 4: *Chemical potential differences along the line x_{Ti}=0.5 at 1000 °C (1273 K), calculated with the CVM-IT approximation using the parameters in Table 1.*

shows regions of steep and of flat composition profiles. This may sometimes look as if there was a two-phase field between the two end-regions.

To illustrate the above discussion, let us consider the diffusion couple made of the two limitrophe stoichiometric B2 compounds $Fe_{50}Ti_{50}/Ti_{50}Rh_{50}$, which was annealed at 1000°C for 20 days. The microstructure of the diffusion zone is shown in Fig. 5a, while a composition profile is shown in Fig. 5b. Despite the long annealing time, the inter-diffusion zone turns out to be very small, only about 12 μm. This shows that at compositions close to stoichiometry,

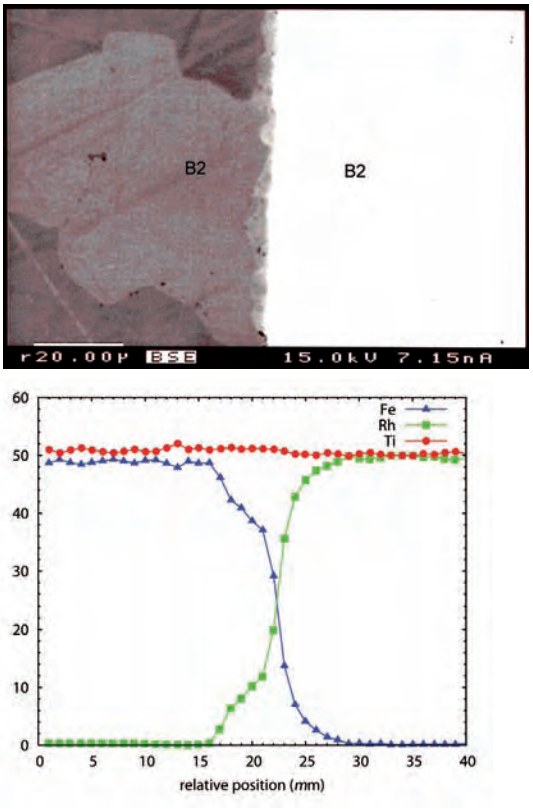

Fig. 5: *(a) Microstructure of the $Fe_{0.5}Ti_{0.5}$-$Rh_{0.5}Ti_{0.5}$ diffusion couple observed by BSE. (b) One EPMA scan crossing the pseudo interface at the diffusion zone between the two B2 grains.*

diffusion within the B2 ordered structure is very slow. Within the section defined by $Fe_{0.5}Ti_{0.5}$-$Rh_{0.5}Ti_{0.5}$, Ti fills one sublattice completely. The Ti-profile turns out constant, while the Fe and Rh composition profiles show steep variations. This can be understood in terms of the variation of the chemical potential differences along this section, shown in Fig. 4. Within the composition interval $0.1 \le x_{Rh} \le 0.45$ the slope of the chemical potential difference $\mu_{Rh} - \mu_{Ti}$ shows only little variation. Therefore, in order to maintain a given driving force for diffusion, i.e. a certain gradient of chemical potential difference, the concentration must vary strongly with distance. This is observed in Fig. 5b. At the very Rh-rich end both potential differences $\mu_{Fe} - \mu_{Ti}$ and $\mu_{Rh} - \mu_{Ti}$ vary strongly with composition providing a high driving force for Fe and Rh diffusion. Here the slope of $\mu_I - \mu_{Ti}$ is positive for $I = Rh$ and negative for $I = Fe$. Both gradients drive Rh diffusion towards the FeTi side of the couple. At the Fe-rich end, $0.04 \le x_{Rh} \le 0.1$, the slope of $\mu_{Rh} - \mu_{Ti}$ is much higher than in the interval $0.1 \le x_{Rh} \le 0.45$. Consequently in this interval the concentration gradient is smaller.

We hope to have shown that the CVM can be applied successfully in explaining diffusion couple features such as pseudo-interface formation and concentration jumps along the profile not associated with phase transformations.

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A Joint 3D-EBSD Crystal-Plasticity-FEM Study of Nanoindentation

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Small scale indentation testing is nowadays an important tool in examining the material response upon the application of localized loading. Nanoindentation is a major method in this field, where hardness is one of the important properties that can be determined by this method. Furthermore, nanoindentation is a major test in the field of thin films. Due to the increased importance of nanoindentation it attracts modellers and experimenters to interpret the measured data in accordance to the deformation mechanisms in the indented zone [1-5]. With an enhanced understanding of indentation mechanics a larger spectrum of constitutive material parameters might be extracted and addressed than before. In that context this study addresses as one particular aspect of nanoindentation the formation of the crystallographic texture and microstructure in the deformation zone around an indent in 3 dimensions. The experiment is conducted on a (111)-oriented Cu single crystal indented with a conical tip to avoid any further symmetry other than that of the crystal structure. The experimental 3D observations are compared to corresponding 3D elastic-viscoplastic crystal plasticity finite element simulations which adopt the geometry and boundary conditions of the experiment. The crystal plasticity finite element simulations are essential for the interpretation of the observed rotation fields. They allow us not only to establish the relationship between crystallographic shear and texture but provide also information about the spatial 3D distribution of the individual shear rates on the active slip systems that entail the observed lattice rotations.

Nanoindents with a depth of about 1μm were conducted on a Cu single crystal using a Hysitron nanoindenter system (TriboIndenter). The indentation direction was in the negative [111] direction of the crystal. The tip used was chosen of conical type to avoid introducing any further symmetry to the experiment rather than that due to the crystal lattice. The EBSD experiments are conducted by using a joint high-resolution field emission SEM-EBSD set-up together with a focused ion beam (FIB) system in the form of a cross-beam 3D crystal orientation microscope (3D EBSD). The FIB was directed normal to the (111) plane producing successive parallel sections as illustrated in Fig.1a. After each milling an EBSD measurement was performed on the new surface (hatched surface in Fig.1b). By the successive milling and measuring operations a 3D image of the crystal misorientation underneath the nanoindent can be constructed. For the detailed nanoindentation setup as well as the experiment with the cross-beam dual microscope refer to [6].

The complexity of the deformation mechanism caused by nanoindentation motivates the use of a crystal plasticity finite element approach for simulating the indentation process. It allows one to investigate the evolution of the material characteristics during the entire indentation process. This includes the active slip systems responsible for the deformation, the change

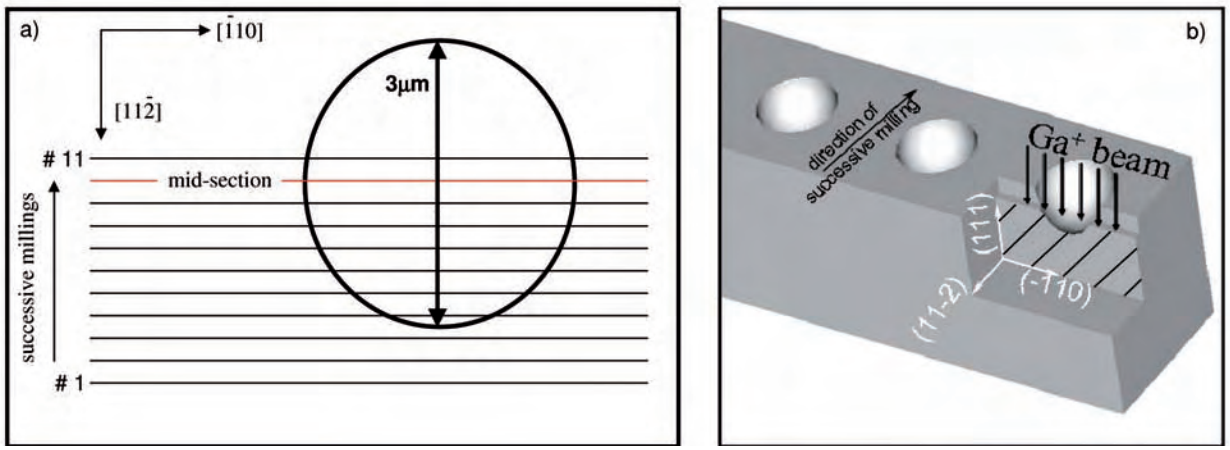

Fig. 1: *Schematic drawing of the geometry of the experiment. a) positions of FIB cuts b) planes of EBSD measurement (hatched plane).*

of the crystal orientation and the pile-up formation at the surface around the indent. Two different material models, namely a phenomenological one and a dislocation density based one, were used in the FE code in order to simulate the experiment.

As phenomenological model the implementation of Kalidindi et al. [7] was used. The constitutive equations used are based on simple power law relations. The hardening law on slip system α is given by

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left| \frac{\tau_\alpha}{s_\alpha} \right|^{1/m} \mathrm{sign}(\tau_\alpha) \qquad (1)$$

where $\dot{\gamma}_\alpha$ is the shear rate on the slip system subjected to the resolved shear stress τ_α having a slip resistance of s_α. $\dot{\gamma}_0$ and m are material parameters representing the reference shear rate and the rate sensitivity of slip respectively. The influence of any slip system β on the hardening behaviour of system α is given by

$$\dot{s}_\alpha = \sum_\beta h_{\alpha\beta} |\dot{\gamma}_\beta| \qquad (2)$$

with

$$h_{\alpha\beta} = q_{\alpha\beta} \left[h_0 \left(1 - \frac{s_\beta}{s_s} \right)^a \right] \qquad (3)$$

where h_0, a, and s_s are slip hardening parameters, which are assumed to be identical for all 12 fcc slip systems used in the simulation. The parameter $q_{\alpha\beta}$ is taken as 1.0 for coplanar slip systems and 1.4 otherwise.

The dislocation density based model introduced in [8, 9] adopts the Orowan equation

$$\dot{\gamma}_\alpha = \rho_{M\alpha}\, b\, v_\alpha \qquad (4)$$

as kinetic equation of state. The mobile dislocation density $\rho_{M\alpha}$ and their velocity v_α are computed as function of the statistically stored dislocations ρ_{SSD}. The evolution of the statistically stored dislocations is formulated in the form of rate equations

$$\dot{\rho}_{SSD} = \dot{\rho}^{+1} + \dot{\rho}^{+2} - \dot{\rho}^{-1} - \dot{\rho}^{-2} \qquad (5)$$

and is regarded as the source of the material hardening.

Here b is the burgers vector and $\dot{\rho}^{+1}$ and $\dot{\rho}^{+2}$ are the production rates of ρ_{SSD} due to the interaction with forest dislocations and dipole formation respectively. $\dot{\rho}^{-1}$ and $\dot{\rho}^{-2}$ are the non-thermal and thermal annihilation rates of the dislocations respectively. For the details of these equations and their derivation refer to [8,9]. As the experiment is being accomplished at room temperature the thermal annihilation is neglected in this study.

The evolution equations involve a number of material parameters which need to be experimentally determined. For the determination of the proper values of the material parameters in each model a compression test of a copper single crystal cylinder was used. The compression axis was in the [111] crystal direction as for the indentation experiment. A very good agreement between the simulated and experimental stress-strain curve could be achieved for both models. Table 1 summarizes the parameters determined for both models during the fitting process of the compression test. However, as the scale of the two experiments (compression, nanoindentation) differs largely and neither of the models includes size effects (the dislocation density based model was used in the form without geometrically necessary dislocations), the fitted values should only be used as a guideline for the selection. In this case we found that choosing a higher initial dislocation density of about 10^{12} m^{-2} results in a better reproduction of the force-depth curve of the nanoindentation experiment.

The finite element code MARC is used to implement the above discussed constitutive models via the user-defined subroutine HYPELA2 [10]. The mesh used consists of 4312 elements and 5224 nodes (Fig. 2). The elements are of 3D-hexahedral type with 8 integration points. Near the centre of the indented area a denser mesh is used due to the expected heavily distorted elements in this zone. The lower face of the cylinder is kept fixed. Otherwise, each node possesses three translational and three rotational degrees of freedom. The tip with a radius of 1.5 μm was modelled as a rigid body. The simulation was performed with displacement controlled motion up to an indentation depth of 1μm in the negative [111] direction. The friction between the indenter and the sample was neglected.

Table 1: *Parameters used for the models (c_1 - c_6 are dimensionless numbers).*

Phenomenological model	Physically-based model	
h_0 = 200 MPa	c_1 = 0.1	(for passing stress)
a = 1	c_2 = 2	(for jump width)
s_s = 75 MPa	c_3 = 0.3	(for obstacle width)
m = 0.012	c_4 = 27	(for lock forming rate)
s_o = 8 MPa	c_5 = 0.04	(for dipole forming rate)
$\dot{\gamma}_0$ = 0.001	c_6 = 50	(for athermal annihilation rate)
	ρ_0 = 5×10^{10} [m^{-2}]	(for initial dislocation density)

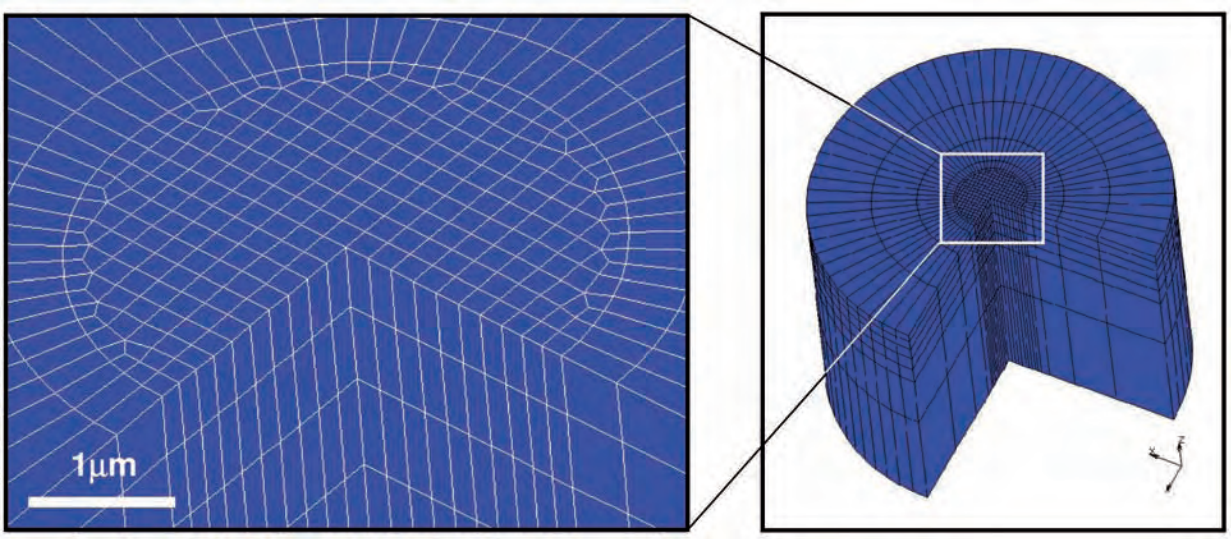

Fig. 2: *FEM mesh used for the simulations.*

The measured crystal orientations were used to obtain the rotation angles of the crystal about the [11-2] crystal direction. The according rotation maps are plotted on the (11-2) sections in the middle column of Fig. 3 at different distances from the centre section of the indent. The maps reveal a pronounced lattice rotation below the indent and lower magnitudes of deformation at the sides of the indent. The measurements show also frequent and rapid changes in the sign of the rotation direction along and near the surface. These changes in the rotation direction diminish with further penetration inside the material. Compared with the experimental findings it can be seen that the rotation patterns simulated using the phenomenological model – Fig. 3 first column – reveal also changes in the direction of rotation. However the model fails to predict the fine details of the deformation-induced rotation patterning. On the other hand the model based on dislocation densities – Fig. 3 last column – succeeded

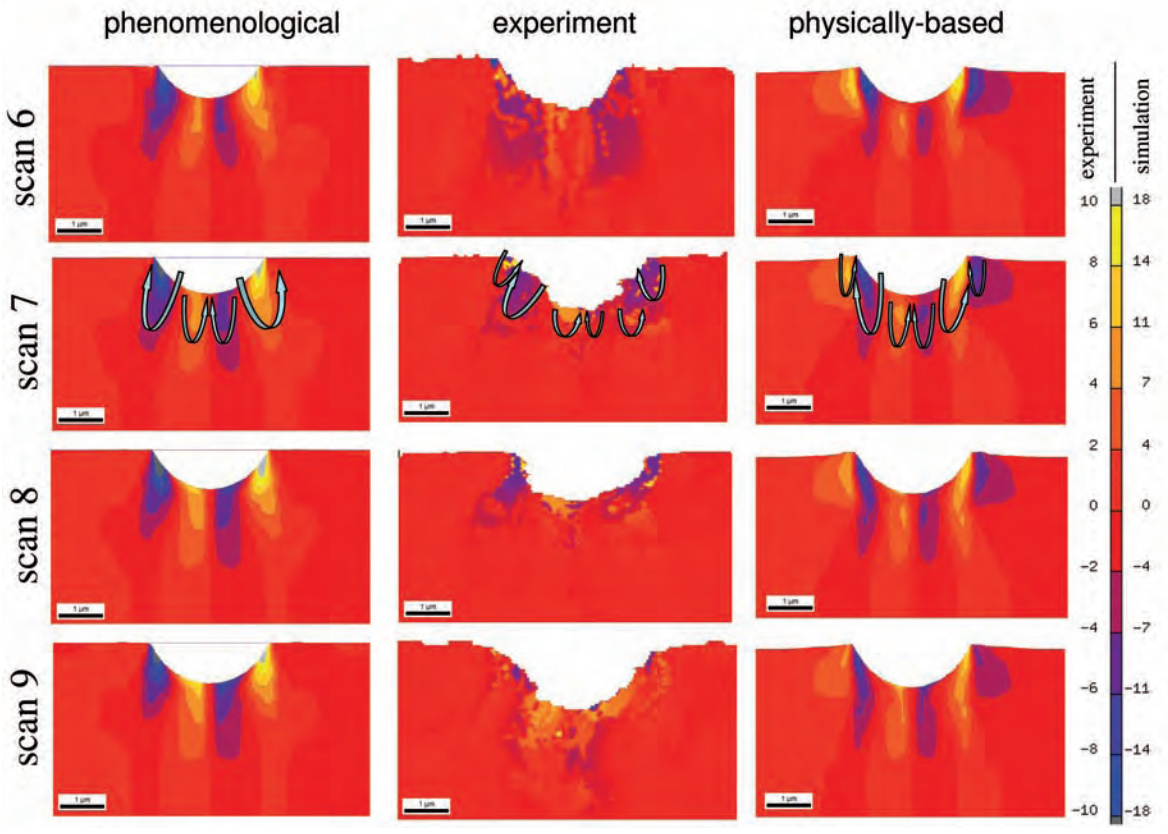

Fig. 3: *Misorientation in degree for simulations and experiment plotted at different cutting positions. The arrows indicate the directions of rotation.*

in capturing finer details of the rotation patterning than the elastic-viscoplastic model. Concerning the absolute values of the rotation angles a maximum rotation angle of 10° could be measured. The calculated maximum rotation angles extracted from the phenomenological and physically-based models are 24° and 23° respectively. This overestimation could be due to edge effects and milling-induced curvature caused by the ion beam, which let the EBSD method miss the measurement at the regions mating the upper surface, where maximum values of rotations are expected.

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Computational Modeling of Microcrack Nucleation using a Physically Based Finite Element Crystal Plasticity Model of Experimentally Characterized Microstructures

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The mechanical failure of engineering materials has historically been evaluated through continuum fracture mechanics, which typically assumes that a crack/flaw initially exists. However, there is much less understanding of how such flaws originate in an otherwise flawless material, particularly at grain (or phase) boundaries of structural metals and alloys. Experimentally, there are some semi-quantitative correlations between damage nucleation and grain boundary (GB) energy (i.e. boundary structure as described by coincidence site lattices, designated as Σ GBs [1-3]). Atomistic methods have been used to develop cohesive energy functions that allow GBs to open up based upon evolving local stresses in FEM models [4,5]. The current paradigm regarding damage is that it is correlated with regions of heterogeneous strain, which is commonly located at or near grain boundaries.

An important element of damage at interfaces depends on the ability to transfer slip across the boundary. Three conceptual requirements for slip transfer have been identified by Clark *et al.* [6] and verified recently in atomistic simulations [7]: 1) activated slip planes in adjacent grains need to be roughly coplanar, 2) residual dislocation content left in the boundary should be small, and 3) the shear stress on the outgoing slip system should be large. These ideas can be quantified using the angles indicated in Fig. 1. While geometric expressions are valuable for identifying slip transfer, they are not necessarily insightful for predicting damage nucleation.

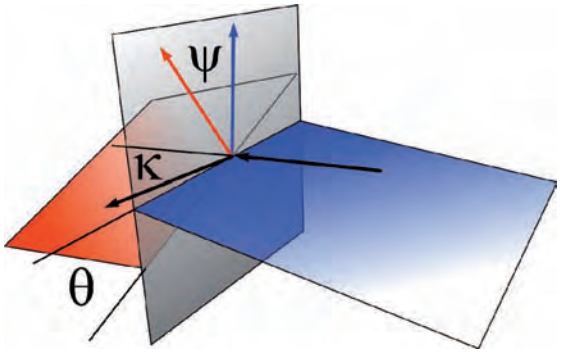

Fig. 1: *Angles used to evaluate the geometrical efficiency of strain transfer (along black arrows on blue and red plane) at a grain boundary (shaded gray).*

Recent experimental assessment of microcrack nucleation in GBs in a model TiAl alloy identified a possible approach for predicting evolution of the GB strength. As TiAl has a limited number of slip and twin systems it was possible to characterize the activated slip and twinning systems with greater ease than, e.g., in a high ductility cubic metal. From this analysis, a fracture initiation parameter (*fip*) gives a definition of GB character (strength) based on interactions of slip systems as activated by a global stress state [8-10]:

$$fip = m_{tw} \left| \hat{\mathbf{b}}_{tw} \cdot \hat{\mathbf{t}} \right| \sum_i \left| \hat{\mathbf{b}}_{tw} \cdot \hat{\mathbf{b}}_{i,ord} \right|$$

This parameter is based on the orientation of the grains and slip systems on both sides of the boundary and the direction $\hat{\mathbf{t}}$ of the macroscopic tensile stress. For GBs with a normal stress component greater than 80% of the applied stress, the *fip* can distinguish between weak and strong GBs with statistical significance [10]; $\hat{\mathbf{b}}_{tw}$ is the Burgers vector for the twinning system with the highest Schmid factor, m_{tw}, in a grain pair, and $\hat{\mathbf{b}}_{ord}$ are Burgers vectors for available ordinary dislocation systems; all expressed in the sample coordinate system. The *fip* value is high when there is much opportunity for imperfect slip transfer, suggesting that (sessile) partial dislocations left in the boundary raise its interfacial energy and facilitate cracking. In contrast to slip transfer parameters, this *fip* incorporates the stress directions and degree of activation of slip systems as a key component.

The material analyzed in this paper has been described in a prior study, a Ti-47.9Al-2Cr-2Nb alloy with duplex microstructure deformed in 4-point bending to a surface tensile strain of about 1.4% [8]. Microstructures surrounding 11 microcracked and 11 intact γ-γ GBs with apparently similar geometrical character were analyzed. One of these regions shown in Fig. 2 (next page), i.e. an intact boundary between grains 13 and 16, and a nearby microcracked boundary between grains 14 and 15, is modeled with a FEM model to assess the following issues: 1) did microcracks develop where the stress or strain was maximized? 2) is the local state of stress different from the global state of stress? 3) how sensitive are modeling results to variations in the FEM mesh or boundary conditions?

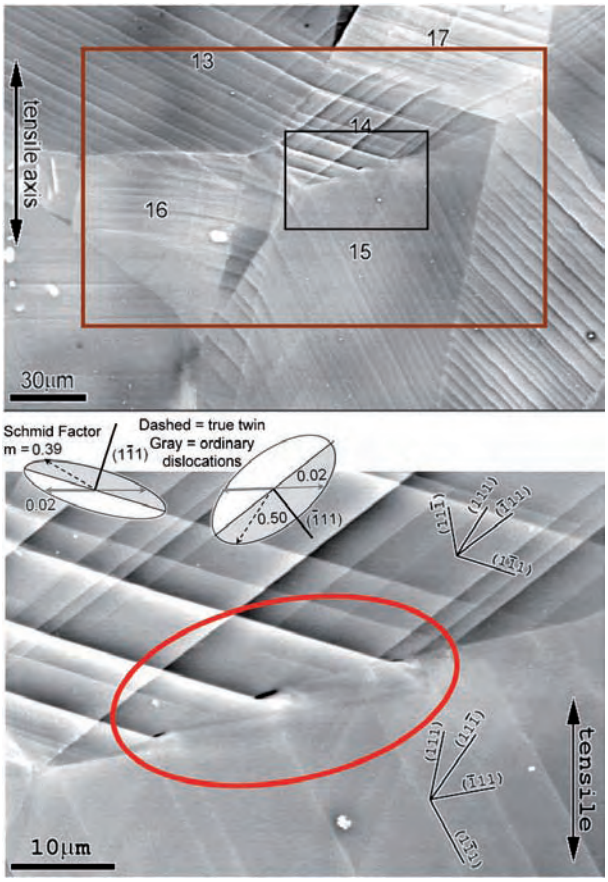

Fig. 2: *An intact boundary between grains 13 and 16, and microcracks formed between grains 14 and 15. The microstructure within the larger box in the upper figure was modeled with a FEM mesh; the smaller box is enlarged to show three microcracks correlated with twin intersections.*

Two FEM meshes were used to represent the grain shapes within the larger box in Fig. 2(a). A simplified (quasi 2D) representation with all GBs parallel to z (Fig. 3a) and a more accurate (3D) representation in which measured GB inclinations from serial sectioning were used [10] (Fig. 3b). The enclosing microstructure was simulated with surrounding elements illustrated in the quasi 2D mesh using the ϕ_1,Φ,ϕ_2 = 90°,90°,0° orientation (they are removed in the 3D mesh to reveal boundary inclinations). This orientation provided symmetrical slip behavior with respect to the loading along the vertical y-direction, was slightly softer than average, but imposed resistance to shear of the vertical boundaries with the modeled microstructure. Boundary conditions were imposed with zero vertical displacement on the bottom edge, and a tensile face load on the top edge. In some runs, the rear surface was pinned in the z (out of plane) direction to constrain displacements that would be imposed by material beneath the modeled volume, but more strongly than would be expected in the real material.

The constitutive description of the material is based on a crystal plasticity formulation using the multiplicative decomposition of the total deformation gradient and taking into account the anisotropic elastic constants [11,12]. Both dislocation slip and mechanical twinning are incorporated as bidirectional and unidirectional slip systems, respectively. The evolution of the deformation resistance for both mechanisms was formulated using a phenomenological hardening matrix. Time integration uses a semi-implicit procedure. MSC/Marc served as FEM framework in which the above outlined model was implemented.

Upon simulated loading to ~1.8% engineering strain, Fig. 4 shows the von Mises stress (left side) and the equivalent total strain (right side) in the quasi 2D (top) and 3D (bottom) models. On the back side, the patterns of stress and strain were roughly similar, but different in detail due to the anisotropy of the elastic and plastic behaviors. Similar plots (not shown) of only the y component of stress and strain look very similar to the equivalent stress and strains presented, indicating that the local stress-strain state is close to the global state.

In Fig. 4, most of the GBs (identified with white lines) developed large stresses, but not in a uniform

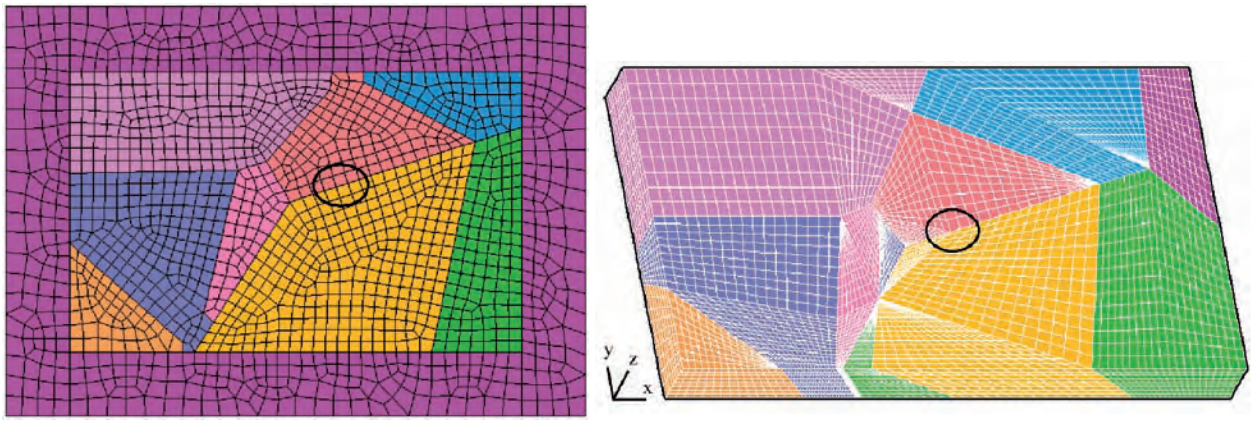

Fig. 3: *Quasi 2D and 3D meshes used to model the TiAl microstructure. Ellipses indicate the location of observed microcracks.*

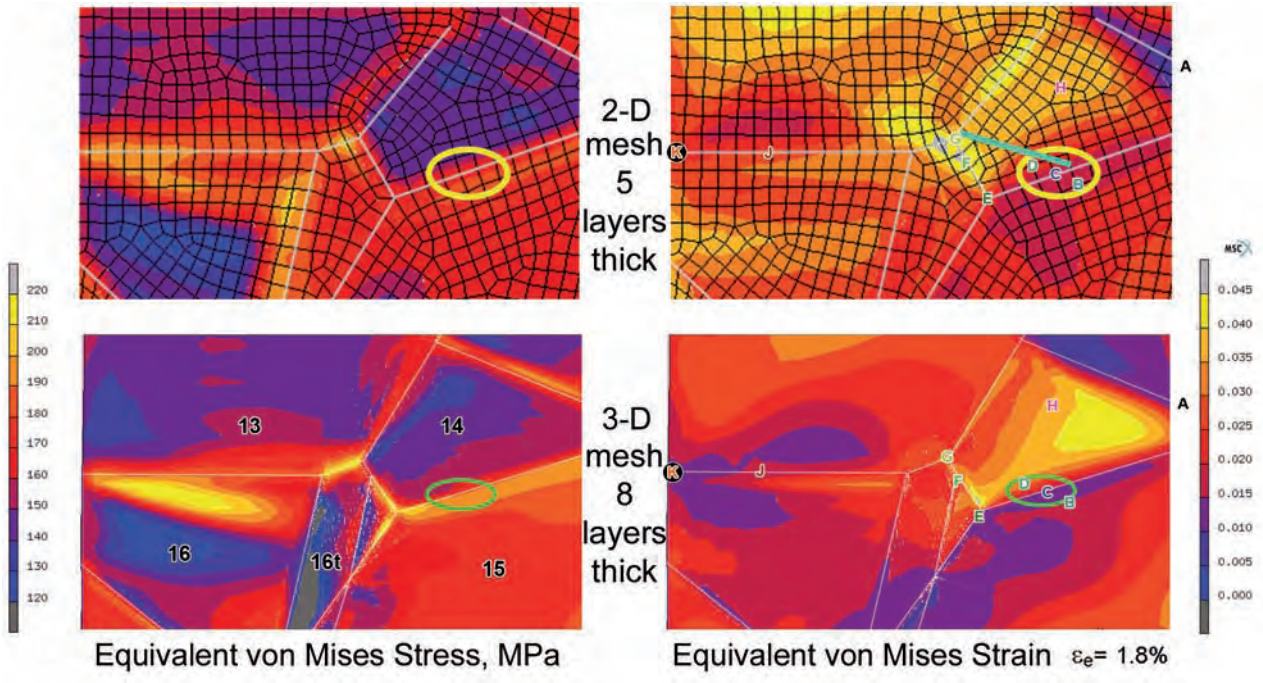

Fig. 4: *Cropped sections of the FEM model illustrating the distribution of stress and strain in the microstructure. White lines indicate GBs in the model, and the ellipses indicate the location of microcracks in the experiment. Local stress-strain for lettered locations is in Figure 5 (K is on back side).*

manner. Similarly, the local strain *varies greatly,* consistent with the experimental observations (note variations in slip trace effects in Fig. 3, which are mostly twins but some dislocation slip bands are also present – they are typically less distinct than twins). The overall patterns of stress and strain are roughly similar in the quasi 2D (top) and 3D (bottom) models. They differ in detail in the regions where the geometry was different, such as in the middle, where annealing twins in grains 16 and 15 were more accurately rendered in the 3D model. This shows that modeling microstructural detail is very important, and needs to be carefully done in regions where critical events take place. However, the stress and strain values are quite similar along the two horizontal GBs, particularly on the surface where microcracks were observed.

The strains and strain *gradients* on the surface (Fig. 4 right side) are maximized near, but not at, the observed location of the microcracks (node C); a local strain maximum occurred at a location along a different boundary 5-10 elements away from the actual crack nucleation sites (nodes E, F, G). This suggests that large local strains in the real material may have occurred to accommodate strain incompatibilities in order to prevent damage, but the accommodation of this strain concentration led to the need to transmit strain across a neighboring weak boundary, in this case between grains 14 and 15. The largest microcrack in Fig. 2 is at the end of a twin that connects with the location of high strain at a triple point labeled G (green line in Fig. 4). At the microcrack location, the magnitudes of the stress and strain are moderate in comparison to other locations with higher stress and strain (e.g. the 13-16 grain boundary, node J), as indicated in Fig. 5 (next page), which shows stress-strain histories at several nodes in the quasi 2D and 3D models. In fact the accumulated strain and stress in the intact 13-16 boundary at node J was greater than in the cracked 14-15 boundary. The stress-strain history where the microcracks were observed (blue heavy dotted line) exhibits neither a relatively high stress nor a high strain. While the details of the stress-strain histories differ in the quasi 2D and 3D models, the relative stress strain behaviors at the tracked nodes are quite similar.

This result is not inconsistent with the fracture initiation parameter analysis [8-10], which indicates that particular slip interactions in the boundary account for cracking (rather than a simple maximum stress or strain criterion). Thus, a maximum strain concentration may be, at best, a pointer to a neighborhood where damage could nucleate, if there is a combination of grain orientations, slip activity, and boundary misorientation that cause a nearby boundary to become weak.

The FEM results show that altering details of grain geometry and variations in boundary conditions affect details, but not the larger scale effects useful for modeling evolution of strain history that could affect damage nucleation. This tentatively suggests that simple representations of microstructures may be sufficient for modeling shears on various slip

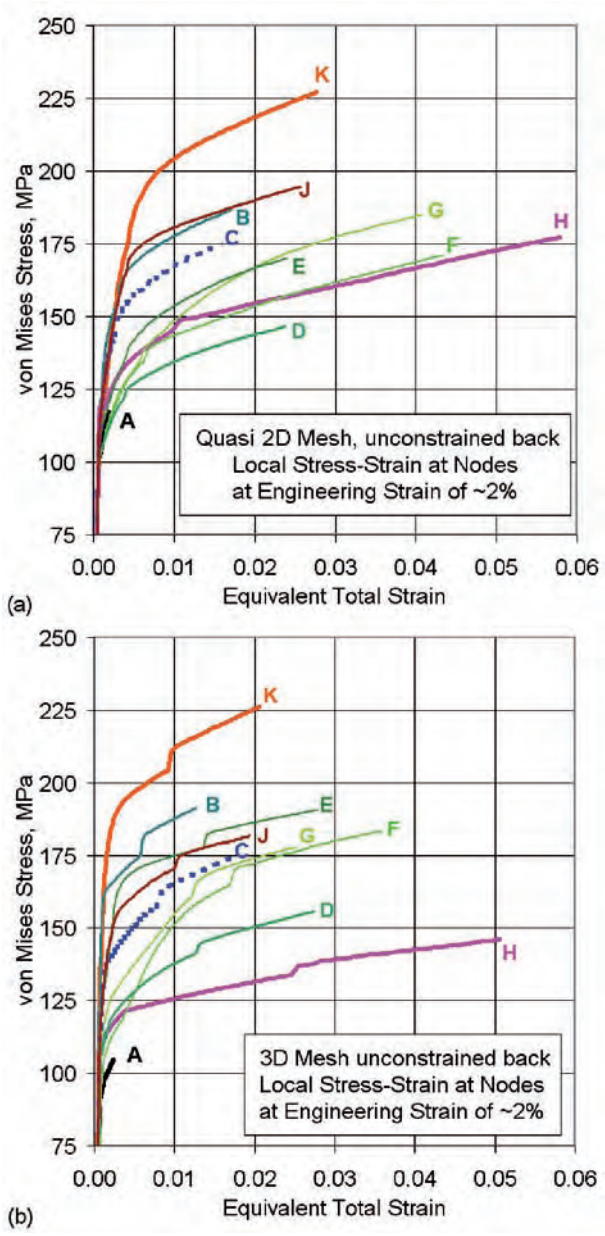

Fig. 5: *Local Stress-strain history of nodes in specific locations in the model indicated in Fig. 4, near the grain 16 twin (green), and near the observed microcrack (blue) (K is on the back side).*

systems with crystal plasticity FEM calculations that are needed to evaluate the *fip* along boundaries. Consequently, this analysis suggests that the *fip* parameter may be a robust parameter, because the local stress and strain obtained from the FEM analysis is not dramatically different from the stress state assumed in the existing *fip*.

Future work will examine if similar conclusions can be drawn from other microstructure models of regions where microcracks developed. In addition, it will be desirable to consider how to express the *fip* as an evolution parameter, as FEM models provide the evolution of shear strains on each slip system, which could be used to extend and sharpen the ideas expressed rather simply by the existing *fip*.

In conclusion, a finite element model of one of the microstructures from a database used to develop a fracture initiation parameter (*fip*) for GB microcracking showed that the local stress-strain conditions are rather close to the simplified global ones. Furthermore, the FEM model showed that microcracks developed in a region of microstructure where the stress-strain history was modest, lending credence to the ideas behind the *fracture initiation parameter*, which is based upon specific slip interactions at a boundary rather than a maximum stress or strain criterion that dominates the current paradigm for predicting damage nucleation.

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Computational Modelling of Thiol Monolayers on Gold

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Understanding and controlling polymer delamination at polymer/metal interfaces is a challenge of great technological relevance as it promotes corrosion of the underlying metal. In particular, the electrochemically driven cathodic delamination, which is determined by electron transfer reactions, poses a problem.

However, a systematic investigation of electron transfer reactions at polymer/metal interfaces requires detailed knowledge of the molecular interface structure – which in most cases is not really understood on the atomistic scale.

Hence, in our approach to the problem we combine experimental techniques with atomistic *ab initio* modelling of the structures and reactions occurring in the process. The basic idea is to prepare samples with molecularly well characterized monolayer films (SAMs or LB films) at the buried interface, which are also accessible by atomistic modelling. Thiol monolayers have turned out as an especially suitable model system for studying degradation mechanisms at buried polymer/metal interfaces, as there is a good correlation of the delamination behavior of polymer/thiol-SAM/gold sandwich samples with the electrochemical behavior of the monolayer films.

The formation of SAMs on metals is believed to involve an initial physisorption followed by a slow chemisorption evolution that leads to a dense high coverage phase [1]. The (√3 x √3)R30 structure of alkanethiols on gold (111) and the c(4 x 2) superstructure are experimentally well known. However, the nature of the metal-sulphur bond and the spatial arrangement remain unclear till today. Fig. 1 shows the possible binding sites and illustrates the current confusion in the theoretical literature [2]: Molecular dynamics simulations suggest that sulphur adsorbs preferentially on fcc, hcp or bridge sites, which seem to be isoenergetic and leaving the molecule to diffuse easily on the surface [3]. Density functional studies using a slab model find a preference for the fcc site [4]. This is also supported by Yourdshahyan et al. for various lengths of the alkyl chain and for different coverage regimes [5]. According to Selloni et al. adsorption on the bridge site is most stable [6,7], whereas Hayashi et al. conclude that the bridge site is slightly displaced towards the fcc site [8]. Including relativistic effects it is found that the sulphur atom resides between the bridge and the fcc site [8], which is in agreement with other recent DFT calculations [10,11]. Recent DFT

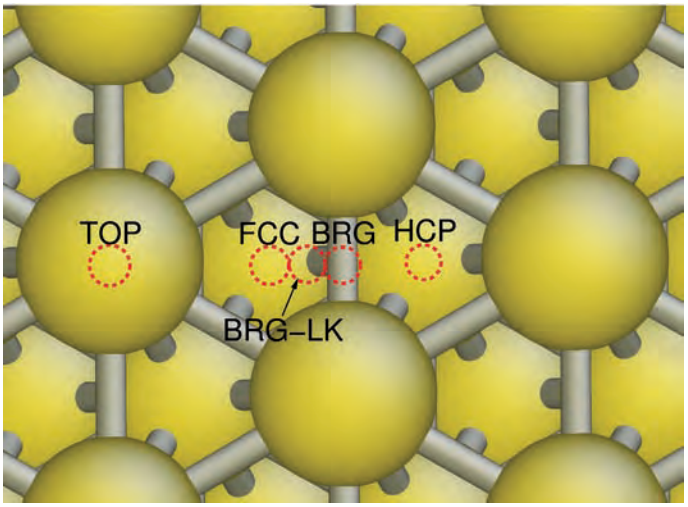

Fig. 1: *Possible binding sites of thiol on Au(111): TOP (top), FCC (face centred cubic), BRG-LK (bridge like), BRG (bridge) and HCP (hexagonally closed packed).*

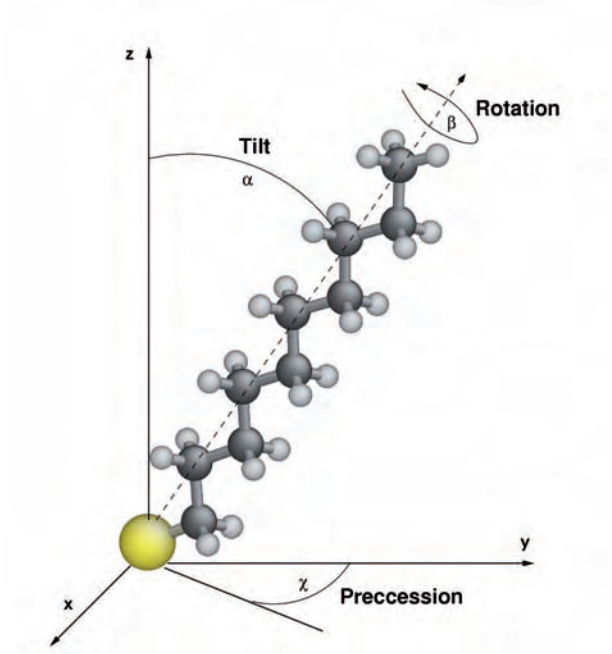

Fig. 2: *Angular degrees of freedom for a thiol molecule on a surface. The surface (not shown) lies in the x-y-plane.*

studies mapping the potential energy surface with the molecule's tilt angle included confirm the bridge site as the favourite [12]. Similarly, there are contradicting experimental reports, surprisingly preferring the top site [13,14], or a combination of bridge and top sites [7,15]. To resolve this issue, we perform atomistic density functional theory (DFT) calculations to model a) the thiol molecules, b) the Au(111) surface and c) a thiol monolayer on Au(111).

Computational method. All DFT calculations where performed in a plane wave pseudopotential approach as implemented in the VASP computer code. DFT exchange correlation contributions are included through the generalised gradient approximation (GGA / PW91). The core electrons were treated by the projector-augmented plane wave method [16] and the valence electrons are described by plane waves with a cutoff energy of 450 eV. For more details see references [17,18].

Mapping the energy surface. As energy differences with respect to binding sites, rotation and tilt angles of the molecules are rather small, finding the global energy minimum is a tedious task and we do not rely on conjugate gradient approaches but map the energy surface. Here not only the three spatial coordinates of the binding sulphur atom enter as parameters, but also the angular degrees of freedom of the molecule. These are shown in Fig. 2, assuming a fully extended all-trans conformation.

The first model system to be investigated is a monolayer of methylthiol – the thiol with the shortest carbon chain – on Au(111). As illustrated in Fig. 3, this system is set up as a periodically repeated unit cell containing an atomically flat (111) slab of gold with the thiol on top. Reciprocal space in the periodic calculation was sampled using a 4 x 4 x 1 Monckhorst-Pack grid with the z-component corresponding to the [111] axis perpendicular to the gold surface. The unit cell contains 4 Au(111) layers and 24 Å vacuum spacing along the [111] direction.

As the disputed binding sites all lie along the high-symmetry line between the top and the hcp position of the sulphur atom, this line was scanned in a first attempt for a tilt angle of α=0°. Here a position close to the fcc site appears energetically favourable. However, the assumption of the thiol to remain perpendicular to the surface seems rather crude and excludes many high-symmetry structures, where the molecule will be tilted with respect to the surface normal.

Hence we include the tilt angle as a further parameter to be varied and with the displacement along the high symmetry line and the tilt angle as parameters for the plot, we obtain a set of energy surfaces, each of them for a given rotation angle β.

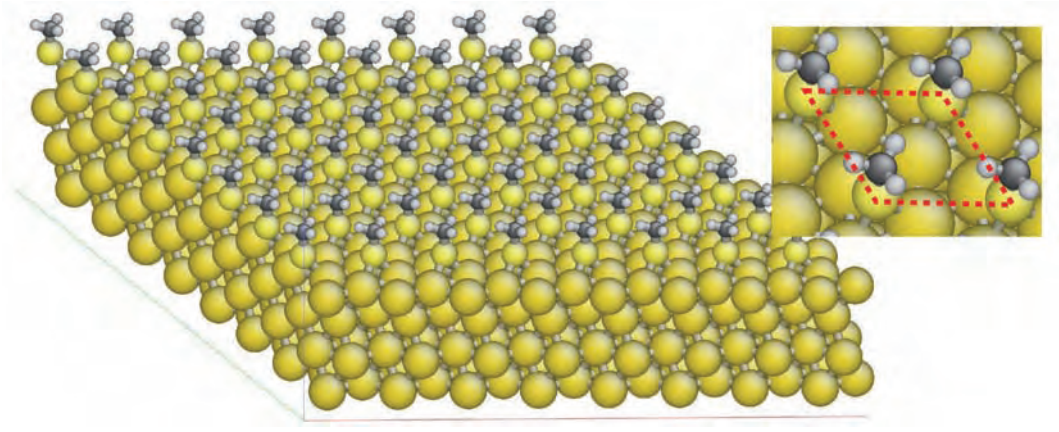

Fig. 3: *Repeated atomistic slab model of a methylthiol SAM on Au(111). The top-right inset depicts the minimum surface unit cell (view along [111]).*

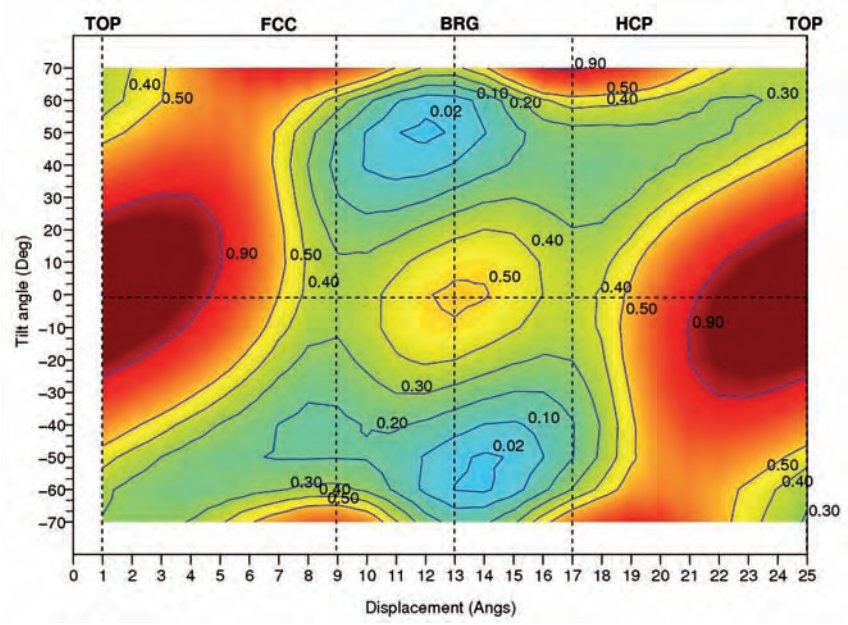

Fig. 4: *Energy surface map of methylthiol on Au(111) for a scan on the high symmetry line between the TOP and HCP binding sites (horizontal axis) with varying tilt angle α (vertical axis). Rotation of the CH_3-head group was set to β = 0°. Energies are given in eV.*

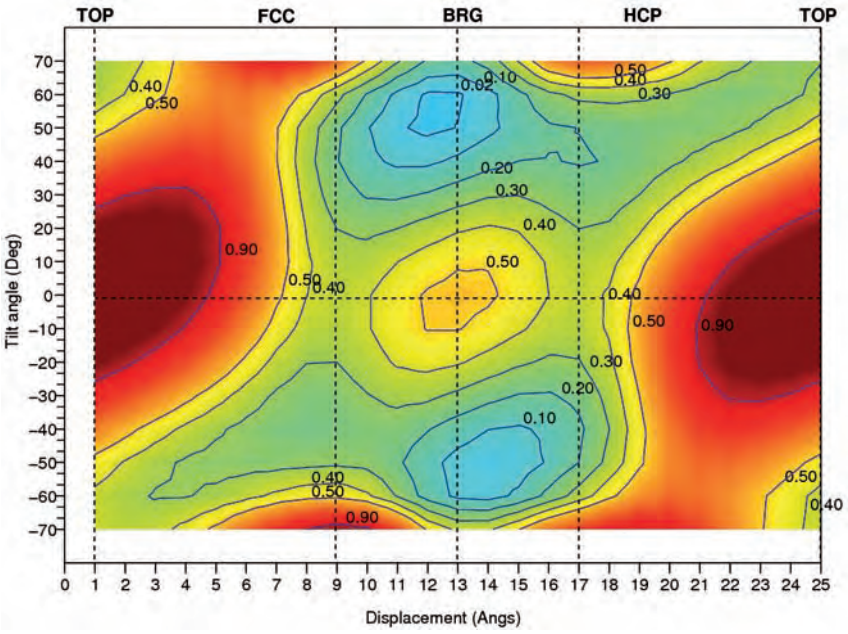

Fig. 5: *Energy surface map of methylthiol on Au(111) for a scan on the high symmetry line between the TOP and HCP binding sites (horizontal axis) with varying tilt angle α (vertical axis). Rotation of the CH_3-head group was set to β = 60°. Energies are given in eV.*

Figs. 4 and 5 give the energy surfaces for β=0° and for β=60°, respectively. Low numbers (blue colours) represent low energies and hence correspond to stable structures.

As can be seen, we find a site close to the bridge site, slightly displaced towards the fcc site to be the energetically preferred site for the sulphur atom of the methyl thiol molecule. In this configuration the molecule is tilted by α~55° with respect to a perpendicular orientation. Tilting the molecule to the other site by the same amount stabilises a bridge site slightly displaced towards the hcp site. The two sites found on the second energy surface differ only by the orientation of the hydrogen atoms. The energy difference between the four structures is marginal.

Rotations of the methyl groups about the C-S axis are generally so fast that they cannot be observed experimentally. On the other hand, the process changing the tilt direction and shifting the adsorption site from fcc-like to hcp-like is predicted to have

a barrier of ~0.45 eV. These two possible sites combined with the 3 equivalent directions on the surface already give 6 different domains for methyl thiol SAMs on Au (111).

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Ab initio Based Modeling of Thermodynamic Properties of Metals

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For a computational design of materials, the key question concerns the identification of the thermodynamically stable crystal structures. The preferred microscopic arrangement of atoms in a well defined crystalline structure depends on the chemical composition of the material and on environmental conditions (e.g. pressure and temperature). For a theoretical modeling of these dependences, the Gibbs free energy is a key quantity. Its minimal value characterizes stable configurations, and the equality of the free energies of two phases indicates phase transitions.

The collection of thermodynamically stable phases in form of phase diagrams is one of the fundamental tools for metallurgists/engineers when determining processing routes (road maps) to design/optimize alloys. Since a mapping of the entire relevant phase space solely by experiment is (for multicomponent systems) extremely time consuming and expensive, approaches such as CALPHAD (CALculation of PHAse Diagrams) have been developed [1]. Based on sophisticated inter- and extrapolation schemes of free energies, these approaches allow the construction of complete phase diagrams using only a few experimental data points. The CALPHAD approach is nowadays a well established and routinely applied tool in materials modeling. Despite its success, a further development and extension of the method with respect to predictive power (e.g. for new alloys/phases), efficiency (e.g. by reducing the experimental input), applicability (e.g. for metastable precipitate phases), and new thermodynamic quantities (e.g. pressure dependence) are crucial. An exciting option, which is pursued in the group “Computational Phase Studies” in the CM department, is to address these issues by supplementing and to some extent replacing the experimental input parameters by employing ab initio computational techniques.

Ab initio methods based on density functional theory (DFT) have continuously improved their performance in predicting material properties without using any empirical parameter or experimental input [2]. First attempts to combine DFT with CALPHAD (e.g. [3,4]) consider in particular the influence of the configurational entropy in compounds. However, ionic vibrations have a substantial influence on thermodynamic properties of materials, too [5]. In recent years it is has become possible to calculate quantities such as phonon spectra, lattice expansions and specific heat from first principles (e.g. [6,7]). This offers the possibility to include even the vibrational entropy in the ab initio determined energies used as an input for CALPHAD. However, the application of this concept requires a careful assessment of the suitability and accuracy of ab initio methods to predict free energies.

For this purpose we made a detailed analysis of DFT results for thermodynamic materials properties. Extremely careful convergence checks were performed, in order to ensure that the remaining error is solely controlled by the choice of the exchange-correlation functional. The accuracies of the standard functionals LDA (local density approximation) and GGA (generalized gradient approximation, here: PBE) were evaluated by comparing them with one another and with experimental data. Finally, the agreement of calculated free energies with predictions of CALPHAD was studied. The focus of this study was on temperature effects due to vibronic contributions. Therefore, only pure (without configurational entropy) and non-magnetic (no magnon-related temperature effects) metals were chosen. In this article, we first focus on aluminum, since it is for theoretical and technological reasons often used as a testbed for thermodynamic modeling [8]. In a second step to discuss chemical trends, results for an extensive set of pure metals which are adjacent to one another in the periodic table of elements and are crystallizing in the fcc (face centered cubic) structure are provided.

Ab initio phonon spectra have been obtained employing the quasiharmonic approximation [9]. Performing supercell calculations, one makes use of the fact that the displacement of an atom out of its equilibrium position gives rise to analytically accessible Hellmann-Feynman forces. The resulting equations of motion of the atoms within a unit cell can be solved analytically and provide the phonon dispersions.

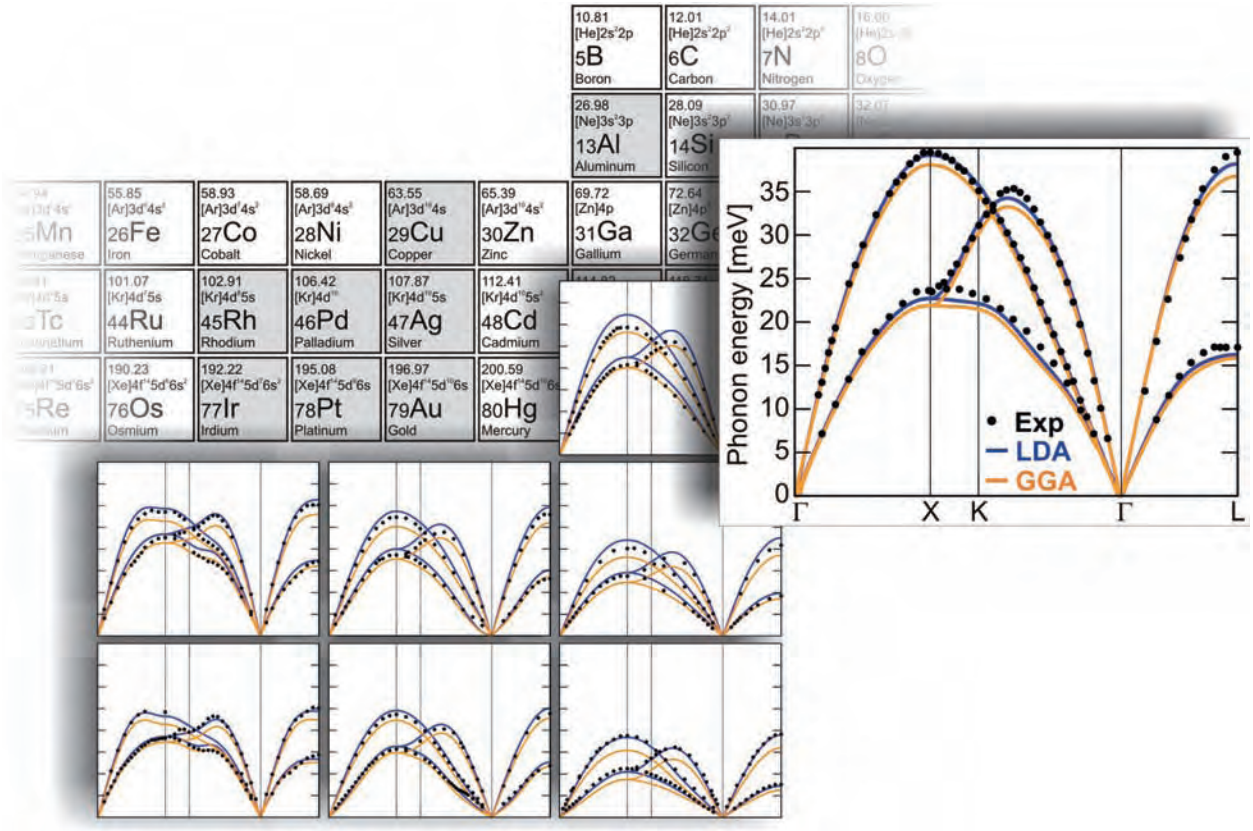

Fig. 1: *Phonon dispersion curves of Al (right) and Cu, Rh, Pd, Ag, Ir, Pt, Au (arranged as in the table of elements). Ab initio results within LDA (blue lines) and GGA (orange lines) are compared with neutron scattering data (dots) [10], using for all elements a coordinate system identical to that of Al. The theoretical lattice constants have been self-consistently chosen such that the temperature corresponds to conditions of the measurements (Al: 80 K, Pt: 90 K, all others: room temperature).*

The phonon spectra in Fig. 1 have been calculated using a supercell, which has 3x3x3 the size of a conventional fcc unit cell. In the case of aluminum (large diagram), the agreement of the ab initio calculation and the experimental data [10] is excellent for all phonon modes. Small deviations are restricted to large (thermodynamically less important) excitation energies and are (as shown in convergence checks) due to the approximations in the exchange correlation functional. Nevertheless, it is a remarkable property of aluminum that the LDA yields nearly the same results as the GGA.

To evaluate whether the excellent agreement is systematic, a detailed study of the phonon spectra of a representative set of metals (see periodic table in Fig. 1) has been performed. Generally, the agreement between theory and experiment for these elements is of almost the same quality as for aluminum. Even modifications of the lattice vibrations due to Kohn anomalies (i.e. the interaction of phonons with the conduction electrons) could be reproduced. Since LDA (GGA) tends to over(under)estimate phonon energies, the small differences of these functionals can serve as error bars.

The thermal expansion, i.e. the change of lattice dimensions with temperature, is another important materials quantity. Within the quasiharmonic approximation it can be obtained by calculating the phonon spectra at several volumes *V*. These lattice excitation energies enter the partition function, providing a temperature-dependent expression for the vibrational entropy [7]. After adding this contribution to the T=0K result of DFT, the Helmholtz free energy *F(T,V)* is obtained. From this function, the thermal expansion can be directly obtained by calculating the volume *V* which minimizes *F* for a given temperature *T*.

The resulting ab initio (i.e. fully parameter free) thermal expansions have been plotted in Fig. 2. Aluminum (large diagram) nicely demonstrates the power of the DFT to accurately describe thermodynamic properties of metals even far away from the temperature regime (T=0K), for which it is traditionally used. A study of the other elements (small diagrams) reveals that the agreement with experiment [11] becomes worse, if the electron occupation number in the d-shell of the transition metals increases.

An interesting observation from these results is that a comparison of LDA and GGA allows an estimation of the predictive accuracy of the thermal expansion: The smaller the difference between these functionals, the better is the agreement with experiments. A more detailed analysis of the difference between LDA and GGA revealed that it is mainly due to errors in the

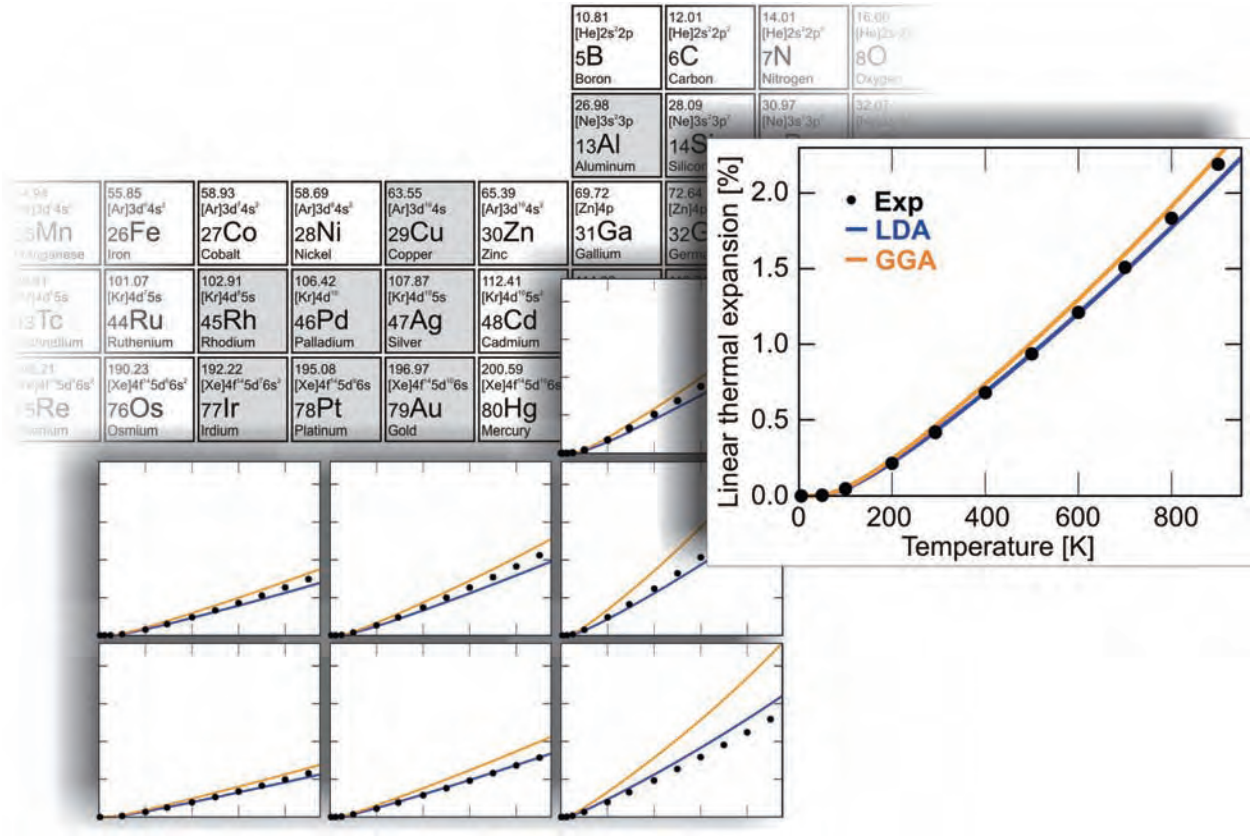

Fig. 2: *Linear thermal expansions of Al (right) and Cu, Rh, Pd, Ag, Ir, Pt, Au (arranged as in the table of elements). Ab initio results within LDA (blue lines) and GGA (orange lines) are compared with experimental data (dots) [11], using for all elements a coordinate system identical to that of Al.*

T=0K potential energy surface. The temperature dependent energy contributions are in excellent agreement with experiment, even if deviations in the phonon spectra are observed. This opens interesting approaches to even improve the accuracy of the DFT calculations.

The Helmholtz free energy *F(T,V)*, like its Legendre transformation, the Gibbs free energy *G(T,p)* is a thermodynamic potential and therefore allows the calculation of a large set of thermodynamic quantities. Instead of discussing all derived quantities, it is worth investigating the reliability of the potential itself. For this purpose, the dependence on the natural variables *V* and *T* is of interest. The volume dependence of the vibrational entropy is described by average Grüneisen parameters, for which a perfect agreement of the ab initio calculations with experiments has been observed.

Particularly interesting is a comparison of the temperature dependence of the ab initio free energy with the results of the CALPHAD method (see Fig. 3). Due to kinetic limitations in low temperature measurements, CALPHAD data are limited to temperatures higher than 200 K for the systems considered in this study. In this temperature regime, the agreement of the ab initio calculation with the results of CALPHAD is excellent. This is not only true for aluminum, but also for all other transition metals included in this study. The agreement is good for LDA and GGA, with a preference for the exchange correlation approximation which best describes the low energy phonon frequencies.

Based on the presented results, we conclude that fully parameter free DFT calculations provide thermodynamic potentials with an accuracy comparable to state of the art empirical schemes such as CALPHAD. We note, however, that demanding investigations, which ensure the convergence e.g. with respect to supercell size or k-point sampling, are needed to reach this accuracy. Remaining limitations are due to the LDA/GGA inherent approximations and are best estimated if the thermodynamic calculations are performed for more than one exchange correlation functional. Having this in mind, the presented techniques can well be used to supplement and/or replace experimental input parameters of CALPHAD, in order to accurately predict thermodynamic materials properties. For an extension of the above described approach to complex compounds further method development is crucial: anharmonic contributions, magnetic excitations and the configurational entropy have to be incorporated into the expression for the free energy. It is the aim of future research in the group “Computational Phase Studies” to develop and

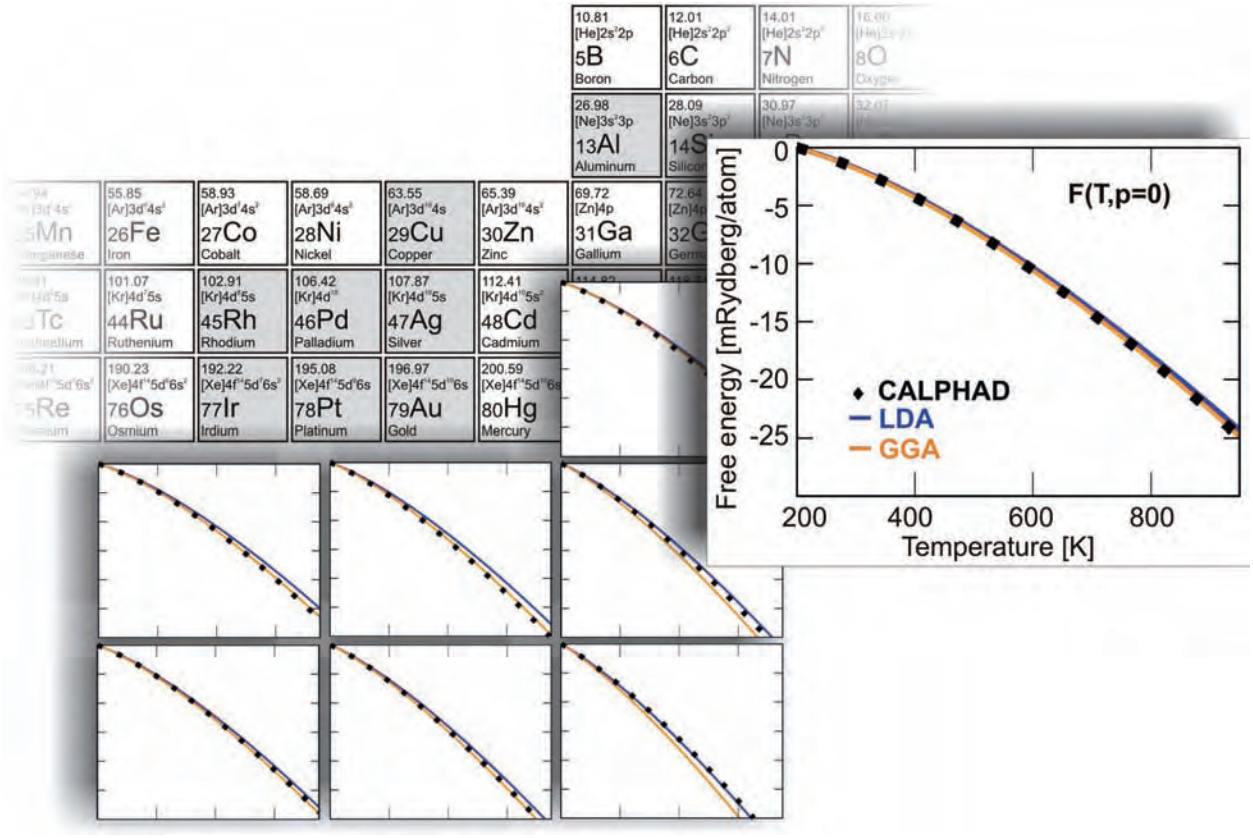

Fig. 3: *Temperature dependence of the Helmholtz free energies of Al (right) and Cu, Rh, Pd, Ag, Ir, Pt, Au (arranged as in table of elements). Ab initio results within LDA (blue lines) and GGA (orange lines) are compared with CALPHAD (Thermo-Calc version Q) calculations (dots), using for all elements a coordinate system identical to that of Al.*

implement efficient ab initio techniques to compute these contributions and to apply them to modern steel alloys.

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The Multi-scale Simulation Library S/PHI/nX

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Department of Computational Materials Design

Multi-scale simulations. Modern material research requires a fundamental understanding of material properties on all scales ranging from the microscopic, via mesoscopic to the macroscopic scale. The microscopic scale describes atomic bond distances, electronic and vibrational properties in the order of Angstroms or fsec. Thermodynamical properties, such as pressure or temperature distributions can be simulated by applying statistical mechanics to reach orders of μm or nsec. Structural properties due to the material's microstructure happen in the mesoscopic scale. Engineering calls for an accurate description in the macroscopic scale to fashion constructions. An important contribution of computational physics to material research and design is the development of highly optimized methods to model accurately the material properties across these scales. Conventionally, different disciplines of computational physics are dedicated to a single scale, respectively. For each scale several highly specialized program packages have been developed from various research teams. As the computer power steadily increases, a new trend of combining the single-scale methods emerges (Multi-scale methods). The large number of single-scale methods and the various approaches to connect them (parameter transfer, embedding, etc.) make the development, implementation and application of such methods rather challenging. A further complication is that single-scale packages consist of lengthy computer codes and are thus hard to maintain. Re-using code fragments across different packages is in practice often not possible.

To address and overcome these issues we have developed a fully object-oriented approach, which allows a seamless coupling of the various single-scale approaches and which provides a platform to easily develop various multi-scale strategies. Although the present implementation bridges only the atomistic scale and the mesoscopic scale the implementational approach is general and allows future developments over all scales. To keep the program code flexible rather than writing a single program which contains all aspects a library – called S/PHI/nX [1] – has been developed. S/PHI/nX relies on a class hierarchy based upon a highly optimized

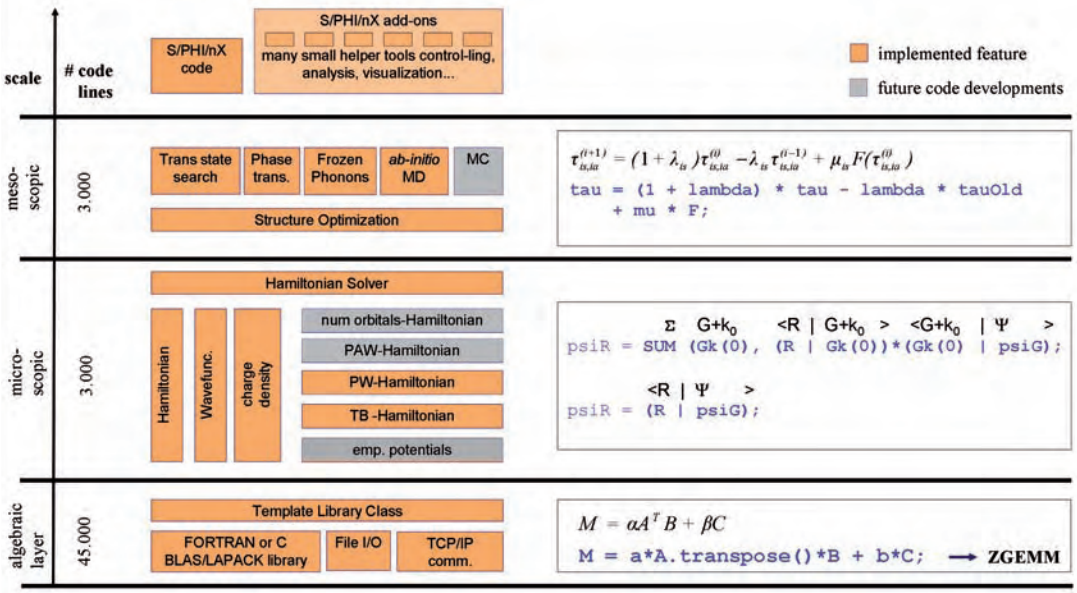

Fig. 1: *Hierarchy of the S/PHI/nX modules. The S/PHI/nX modules are organized in various layers to split up memory management, numerics, and physics. In the bottom layer memory management, file input/output as well as algebraic operations are defined. The microscopic layer introduces the Dirac notation in order to provide an intuitive interface to quantum mechanics. The atomic structure library forms the back-bone of the mesoscopic layer. The high abstraction level of S/PHI/nX allows the development of new algorithms with only a fraction of code lines usually needed. Note, that the microscopic and mesoscopic layer could be defined in less than 10.000 lines while the size of conventional DFT packages is as large as 50.000-150.000 code lines. The code becomes smaller and hence, simpler to maintain. At the same time development of new algorithms can be dramatically accelerated since memory management, algebraic optimization can be shifted from the developer to the compiler.*

algebraic layer (see Fig. 1). Based on this algebra library we have developed modules and interfaces to address the various scales.

The fundamental physical layer of this approach employs density functional theory [2] (DFT), which is a well established, efficient and parameter-free approach to describe the quantum mechanical nature of materials on the atomistic scale. Algorithms in quantum mechanics are often expressed in terms of algebraic equations. On modern computer architectures highly optimized numeric libraries specialized in solving algebraic equations efficiently on the respective platform are available (BLAS/LAPACK). Conventionally, algebraic expressions are transcribed manually into such BLAS/LAPACK function calls in order to achieve high performance. This process is both time consuming as well as error-prone. Hence, only the most important calls are usually optimized. In order to achieve peak performance without having to perform cumbersome hand-optimization, we developed a novel C++ numeric library that automatically performs this task. For example, an algebraic expression

$$\mathbf{M} = a\mathbf{A}^{\mathrm{T}}\mathbf{B} + b\mathbf{C}$$

with the matrices **M**, **A**, **B**, and **C** and scalars *a* and *b* has in S/PHI/nX the following notation

```
M = a*A.transpose()*B * b*C
```

and will be automatically replaced by the compiler with a single LAPACK call. As our mapping is fully automated *all* algebraic equations will be optimized and peak performance is guaranteed (see Fig. 2). At the same time the developer can focus on the physical model rather than on low-level numeric/programming issues.

As a first step, to describe the atomistic scale a density functional theory (DFT) module has been developed on top of the above described fast algebra library. Depending on the system to be modeled different basis-sets are suited to express the Hamiltonian. Chemical bonding of molecules or biological systems is accomplished best by applying atomic or numerical orbitals while periodicity of semiconductors and metallic systems calls for applying pseudo potential plane-waves [3] (PS-PP) or projector augmented waves [4] (PAW). State-of-the-art program packages are usually focusing on only a single basis-set. In S/PHI/nX a new ansatz has been chosen to allow a basis-set free definition of the numerical representation of the Hamiltonian, which allows the choice of the best fitting basis-set for the system under consideration. This ansatz is based on the Dirac notation. Similar to the algebra library the compiler replaces the abstract Dirac operators with the actual projector functions. To be more specific, let us consider as an example the computation of the density in real space of an atomic orbital $|\mu\rangle$ given in a plane wave basis set:

$$|\Psi(\mathbf{R})|^2 = \left|\sum_{\mathbf{G}} \langle \mathbf{R}|\mathbf{G}\rangle\langle \mathbf{G}|\mu\rangle\right|^2$$

This expression can be expressed in S/PHI/nX by simply writing:

```
psiR2 = SUM(G,  (R|G) * (G| mu) )^2
```

The result is visualized in Fig. 3. Therefore, when developing or testing new algorithms or approaches the developer can focus on the actual algorithm while the compiler takes care of the physical implementation, optimization of algebraic expressions and memory management. Thanks to this abstraction level quantum mechanical algorithms can be implemented and tested within a fraction of the time used in conventional methods. For example, the implementation of an *ab-initio* based self-consistent tight-binding [5,6] (SC-DFTB) schema in S/PHI/nX has been implemented within weeks instead of months or years.

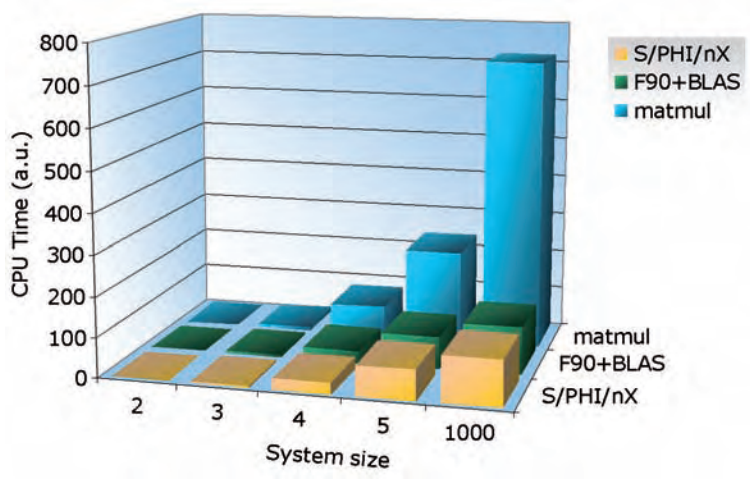

Fig. 2: *Performance results of matrix operations using the S/PHI/nX library, hand optimized Fortran90 code and the generic F90 matmul function. The resulting S/PHI/nX executable is as fast or faster than the manually optimized Fortran code.*

The basis-set free DFT layer of S/PHI/nX is connected to an atomic structure library, which is capable of performing structure optimization, molecular dynamics as well as transition states computations. This library provides access to dynamic matrices used to determine thermodynamic potentials via evaluation of phonons.

In conclusion of this part, the S/PHI/nX approach developed by us provides an excellent basis for a rapid development of computationally highly efficient multi-scale algorithms.

Multi-scale visualization. S/PHI/nX computations, which aim at performing computations at various length and time scales, call for an integrated visualization over all relevant scales. One example are DFT calculations, which are restricted to only few hundred atoms but generate huge datasets such as wave functions, charge densities, or potentials. When empirical potentials are employed instead of ab-initio based potentials up to several million atoms have to be visualized. Mesoscopic simulations as needed e.g. in the metal forming (department of Prof. Raabe) require mainly the visualization of high dimensional vector fields. For example, seven-dimensional vector fields are used to display the experimentally obtained grain distributions and orientations. Here typical mesh sizes are of the order of 1.000x1.000x200. Macroscopic descriptions generate stress and tension fields of similar dimensions. Thus, in various scales very different entities have to be visualized with highest performance. A detailed analysis showed that present tools are neither flexible/universal enough nor sufficiently fast to visualize the huge amount of data. We have therefore initiated the development of a visualization tool – called PHInaX [7] – which allows to overcome these limitations.

The visualization engine of PHInaX is based on highly specialized OpenGL extensions. With standard graphic cards (e.g. nVidia) we are able to visualize systems consisting of 1.000.000 atoms with a performance of more than 3 frames per second. To achieve a comparable frame rate commercial products (such as Materials Studio [8]) have to be limited to 50.000 atoms. PHInaX benefits from current trends in the visualization market. For example, particle systems as often used to render explosions have been implemented to PHInaX to render large scalar fields at similar high performance ratios (see Fig. 4).

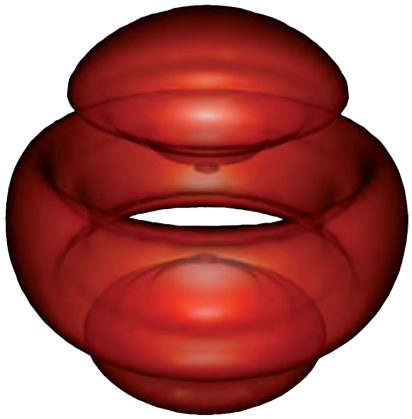

Fig. 3: *Visualization of the result of a single line of S/PHI/nX code "(SUM(G,(R|G)*(G|mu)).absSqr()" for the example of a* d_{z^2} *orbital.*

Both packages, S/PHI/nX and PHInaX, provide a bundle for efficient multi-scale simulations and data analysis. Their modular approaches combined with a high computational abstraction level allow the developer to focus on optimizing algorithms rather than programming and hence, providing a fast simulation and visualization environment.

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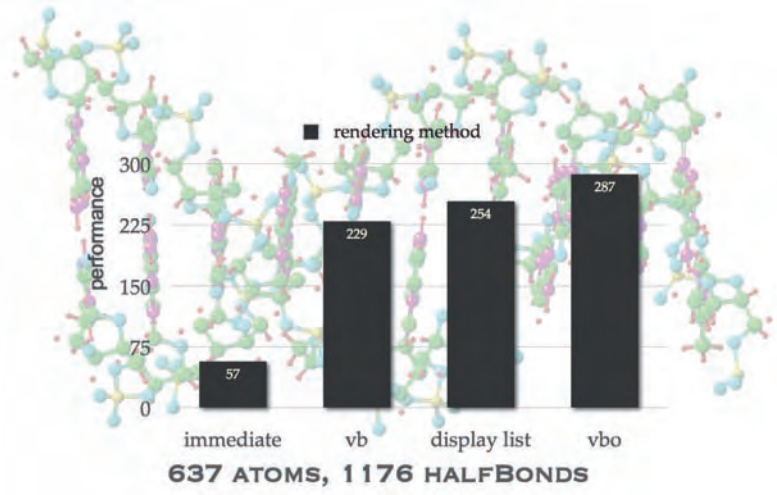

Fig. 4: *The application of various OpenGL extensions can increase the render performance of large data sets dramatically. The resulting performance data are measured by means of rendering a DNA fragment.*

PART IV.

GENERAL INFORMATION AND STATISTICS

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PYZALLA, Anke Rita, Prof. Dr.-Ing. (since Nov. 2005)
RAABE, Dierk, Prof. Dr.-Ing.
STRATMANN, Martin, Prof. Dr.rer.nat.

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HILLERT, Mats, Prof. Dr., Stockholm/Schweden

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

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FROMMEYER, Georg, Prof. Dr.-Ing.	01-01-1983	head of dept.
NEUGEBAUER, Jörg, Prof. Dr.rer.nat.	11-01-2004	director
PYZALLA, Anke Rita, Prof. Dr.-Ing.	11-01-2005	director
RAABE, Dierk, Prof. Dr.-Ing.	07-01-1999	director
STRATMANN, Martin, Prof. Dr.rer.nat.	01-01-2000*	director

*chief executive since 06-01-2002

Scientists at the Institute
(departments in alphabetical order)

Computational Materials Design

Neugebauer, Jörg, Prof. Dr.rer.nat. (*head of department*)

Abu-Farsakh, Hazem, M.Sc.Phys. (*guest*, Jordan), since 07-01-2005

Boeck, Sixten, Dipl.-Phys. *(group head)*

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Dick, Alexey, Dipl.-Radiophys. (Belarus)

Friak, Martin, Dr. rer.nat. (*group head,* Czechia), since 06-01-2005

Grabowski, Blazej, Dipl.-Phys. (*guest*), since 05-01-2005

Hamdi, Ben Ismail, Dipl.-Phys. (*visiting scientist,* Tunisia), 07-01-2005 to 08-31-2005

Hickel, Tilmann, Dr.rer.nat. *(group head)*, since 05-16-2005

Ismer, Lars, Dipl.-Phys., since 04-01-2006

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Marquardt, Oliver, Dipl.-Phys., since 10-01-2005

Petrov, Michal, Mgr. (*guest*, Czechia), since 10-06-2005

Qteish, Abdallah, Prof. Dr. (*visiting scientist,* Jordan), 07-01-2005 to 08-31-2005 and 06-08-2006 to 07-06-2006

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Cerceau Isaac Neta, Augusta, Dipl.-Ing. (Brazil), since 01-01-2006

Coelho, Rodrigo Santiago, Dipl.-Ing. (Brazil), since 03-01-2006

Da Fonseca Barbatti, Carla, Dr.rer.nat. (Brazil), since 01-01-2006

Dzieciol, Krzysztof, Dipl.-Ing. (Poland), since 10-012006

Fernandes de Souza, Dimas Silva, Dipl.-Inf. (Brazil), since 01-01-2006

Juricic, Claudia, Dipl.-Ing., since 10-01-2006

Kostka, Alexander, Dr.-Ing. (*group head,* Poland), since 02-13-2006

Moscicki, Marcin, Dipl.-Ing. (Poland), since 03-06-2006

Pinto Cavalcanti, Haroldo, Dr.-Ing. (*group head,* Brazil), since 03-01-2006

Silva, Pedro Augusto, Dipl.-Ing. (Brazil), since 03-01-2006

Sket, Federico, Dipl.-Ing. (Argentina), since 02-01-2006

Materials Technology

Frommeyer, Georg, Prof. Dr.-Ing. (*head of department*)

Bernst, Reinhard, Dipl.-Phys.

Brokmeier, Klaus, Dipl.-Ing.

Brüx, Udo, Dipl.-Phys., until 08-31-2005

Deges, Johannes, Dipl.-Phys.

Dovbenko, Oleksandr, Dr. (Ukraine), until 12-31-2005

Eleno, Luiz Tadeu Fernandes, M.Sc. (Brazil)

Engberding, Nico, Dipl.-Ing., since 08-15-2006

Fischer, Rainer, Dr.-Ing., until 04-17-2005

Gnauk, Joachim, Dr.rer.nat. (*group head*)

Jiménez, José, Dr. (*guest,* Spain) 01-31-2005 to 02-26-2005, 07-07-2005 to 08-30-2005, 02-20-2006 to 03-17-2006, 07-24-2006 to 09-04-2006, 11-20-2006 to 12-04-2006

Knezevic, Vida, Dipl.-Ing. (Serbia and Montenegro), until 07-31-2005

Konrad, Joachim, Dipl.-Ing. (*50%*), until 01-31-2006

Krein, Ronny, Dipl.-Ing., since 08-01-2005

Maier, Alois, Dipl.-Ing. (Austria), since 04-11-2005

Palm, Martin, Dr.rer.nat.

Pozuelo Alba , Marta, Dr.rer.nat. (Spain), 02-15-2005 to 09-30-2005

Prymak, Oleg, Dr.rer.nat. (Ukraine), since 05-02-2006

Rablbauer, Ralf, Dr.rer.nat. (*group head* since Dec. 2005), since 09-01-2005

Risanti, Doti-Dewi, M.Sc. (Indonesia), until 08-12-2005

Schneider, André, Dr.rer.nat., until 03-31-2005

Sham'oun Raban, Siba Jubrael, Dr. (*guest,* Iraque), 02-05-2005 to 04-20-2005

Siggelkow, Lisa (*guest*), from 10-23-2006 to 11-17-2006

Stallybrass, Charles, Dipl.-Phys., until 05-31-2005

Stein, Frank, Dr.rer.nat.

Strondl, Annika, M.Sc. (Sweden), until 03-14-2005

Wenke, Rainer, Dipl.-Phys.

Wittig, James, Prof. (*guest,* USA), 07-11-05 to 08-05-2005, 06-15-2006 to 07-15-2006

Zeller, Susanne, Dipl.-Ing. (Austria)

Metallurgy and Process Technology

Büchner, Achim R., Dr.rer.nat. (*provisional head of department, group head*), until 07-31-2005

Microstructure Physics and Metal Forming

Raabe, Dierk, Prof. Dr.-Ing. habil. (*head of department*)

Al-Sawalmih, Ali, Dipl.-Phys (Jordan)

Aghajani Bazazi, Ali, M.Sc. (Iran), since 03-01-2006

Ardehali-Barani, Araz, Dipl.-Ing. (Germany and Iran), until 07-31-2006

Balasundaram, Keerthika, M.Sc. (India), since 02-13 -2006

Bastos da Silva, Alice, Dipl.-Ing. (Brazil)

Bieler, Thomas Rector, Prof. (USA), since 01-01-2006

Brahme, Abhijit, Ph.D. (USA), since 11-01-2006

Counts, Art, Ph.D. (USA), since 11-15-2006

Demirel, Melik C., Ph.D. (*guest, AvH fellow,* USA), 05-01-2005 to 05-31-2005

Detroy, Sandra, Dipl.-Ing, until 09-30-2005

Dewobroto, Natanael, Ph.D. (Indonesia), until 10-31-2005

Dorner, Dorothee, Dr.rer.nat., until 10-31-2005

Eisenlohr, Philip, Dr.-Ing., since 03-01-2006

Fabritius, Helge Otto, Dipl.-Biol., since 04-01-2005

Frommert, Matthias, Dipl.-Ing., since 03-15-2006

Godara, Ajay, M.Sc. (India)

Han, Chung-Sook, Ph.D. (Korea), until 06-30-2005

Han, Jun Hyun (Korea), 08-01-2005 to 08-31-2005

Hantcherli, Luc, M.Sc. (France), since 10-01-2005

Hartley, Craig, Prof. (USA), 09-24-2006 to 10-22-2006

Haurand, Hyeon Sook, Ph.D. (South Korea), until 02-28-2005

Hu, Shuiping, Ph.D. (*guest,* China), 10-15-2005 to 10-22-2005

Jia, Juan, M.Sc. (China), until 05-31-2006

Kobayashi, Satoru, Dr. (Japan), until 10-31-2006

Konrad, Joachim, Dipl.-Ing. (*50%*), until 01-31-2006

Liu, Tao, M.Sc. (China), since 05-01-2006

Ma, Anxin, Ph.D. (China), until 05-31-2006

Ma, Duangchen, Master student (China), since 07-01-2006

Mao, Weimin, Prof. (*guest*, China), 10-15-2005 to 10-22-2005

Moss, Matthew Hale, Mat.Eng. (UK), until 02-28-2006

Murty Susarla V.S., Ph.D. (*guest, AvH fellow,* India), 07-01-2006 to 07-31-2006

Nikolov, Svetoslav, Ph.D. (Belgium and Bulgaria)

Ponge, Dirk, Dr.-Ing. (*group head*)

Pramono, Andika, Ph.D. (Indonesia), 10-01-2005 to 12-31-2005

Ramesh, Mageshwaran, M.Sc., from 01-10-2005 to 03-31-2006

Rasp, Wolfgang, Dr.-Ing. (*group head*)

Raue, Lars, Dipl.-Geow., since 02-01-200

Romano Triguero, Patricia,Ph.D. (Spain)

Roters, Franz, Dr.rer.nat. (*group head*)

Sachs, Christoph, Dipl.-Ing.

Sander, Benedikt, B.Sc., since 04-01-2006

Sandim, Hugo, Prof. (*guest,* Brasil), 02-01-2006 to 03-01-2006

Sato, Hisashi, Ph.D. (Japan), until 09-23-2005

Singh Ram Niwas, Ph.D. (*guest, AvH fellow,* India), 01-01-2005 to 07-31-2005

Song, Rongjie, Dipl.-Ing. (China), until 09-30-2005

Takahashi, Tetsuya, M.Sc., (Japan), until 12-09-2005

Thiessen, Richard, Ph.D. (Canada), since 11-02-2006

Tihkhovskiy, Ilya, Dr.-Ing. (Russia)

Tjahjanto, Denny, Ph.D. student (*guest*), 09-01-2006 to 11-30-2006

Torizuka, Shiro, Dr. (*guest,* Japan), 10-09-2006 to 12-22-2006

Varnik, Fatholla, Dr.rer.nat. (Iran and France)

Wichern, Christian, Ph.D. (USA), until 10-31-2005

Winning, Mirjam, Dr.-Ing. habil, since 12-01-2005

Yi, Sangbong, Ph.D. (Korea), until 04-30-2006

Yuan, Lei, Master student (China), since 07-01-2006

Yusupov, Artem, Dipl.-Ing. (Russia), until 06-30-2006

Zaafarani, Nader, M.Sc. (Egypt)

Zaefferer, Stefan, Dr.-Ing. (*group head*)

Zambaldi, Claudio, Dipl.-Ing.

Scientific Honours

Dipl.-Ing. A. Ardehali Barani and Dr. D. Ponge received the “Stahl-Innovationspreis 2006” in the category “Research and Development” of the Steel Institute VDEh for the development of a new technology for the production of high strength spring steels for automotive applications.

Dipl.-Phys. R. Bernst, Prof. Dr.rer.nat. G. Inden and Dr.rer.nat. A. Schneider received the Best Poster Award at the Calphad XXXV Conference in Haifa/Israel (May 7-12, 2006) for their poster ‘Carburization of Fe-X (X=Si, Mo, V) Diffusion Couples’.

Prof. Dr.-Ing. G. Frommeyer became member of the Jury of the “Eugen-und-Ilse-Seibold-Preis 2007” of the DFG, Aug. 2006.

Prof. Dr. H. J. Grabke received the IMR-SAS Award of the Institute for Materials Research (IMR) of the Slovakian Academy of Sciences, Košice, Slovakia, on the occasion of the 50th anniversary of the IMR for his important contributions to the achievements of the IMR in scientific research, industrial development and economic cooperation, 2005.

Prof. Dr.-Ing. habil. G. Grundmeier was appointed Full Professor for “Technische Chemie” at the Universität Paderborn after successful habilitation at the Ruhr university Bochum on July 7, 2006 with the habilitation thesis “Interface Analysis and Engineering of Thin Functional Films on Metals” (2006).

Dr.rer.nat. A.W. Hassel was elected Fellow of the International Center for Young Scientists at the National Institute for Materials Science, Tsukuba, Japan (2005).

Dr.rer.nat. A.W. Hassel was appointed associate editor of the journal Science and Technology of Advanced Materials (2006).

G. Klimow, Dipl.-Chem. K. Wapner and Dr.-Ing. G. Grundmeier received the 2nd Best Poster Award for their poster **“**Applications of a Scanning Kelvin Probe for Studying Modified Adhesive/Metal Interfaces under Corrosive and Mechanical Load”, 3rd World Congress on Adhesion and Related Phenomena (WCARP-III), Beijing, China, October 2006.

Dr.-Ing. J. Konrad received the “First Price Niobium-Student Research Award” of the Institute of Materials, Minerals and Mining funded by the Niobium Product Comp., May 2006.

Dipl.-Chem. K.A. Lill, Dr. K. Fushimi, Dr.rer.nat. A.W. Hassel and M. Seo received the Best Paper Award for the Talk ”Investigations on the kinetics of single grains and grain boundaries by use of Scanning Electrochemical Microscopy (SECM)”, 6th International Symposium on Electrochemical Micro & Nanosystem Technologies, Bonn, Germany, August 2006.

Dipl.-Chem. K.A. Lill, Prof. Dr.rer.nat. M. Stratmann, Prof. Dr.-Ing. G. Frommeyer and Dr.rer.nat. A.W. Hassel received the Best Poster Award for their poster ”Investigations on anisotropy of nickelfree alloys with combined local and trace analysis”, GDCh Annual Meeting 2005, Section Applied Electrochemistry, Düsseldorf, Germany, October 2005.

Ph.D. A. Ma, Dr.rer.nat. F. Roters and Prof. Dr.-Ing. D. Raabe published two papers holding ranks No. 10 and No. 12 among the 25 most downloaded papers of Acta Materialia in 2006 (rank 10: “On the consideration of interactions between dislocations and grain boundaries in crystal plasticity finite element modeling - Theory, experiments, and simulations” in vol. 54, pp. 2181-2194, and rank 12: “A dislocation density based constitutive model for crystal plasticity FEM including geometrically necessary dislocations” in vol. 54, pp. 2169-2179).

Dr.-Ing. S. Milenkovic and Dr.rer.nat. A.W. Hassel received the Best Poster Award for their poster”A combined method for the production of self-organised metallic nano-structures”, 6th International Symposium on Electrochemical Micro & Nanosystem Technologies, Bonn, Germany, August 2006.

Prof. Dr.rer.nat. P. Neumann, director emeritus of the Max-Planck-Institut für Eisenforschung, was awarded the honorary degree Doctor honoris causa of the Friedrich-Alexander-Universität Erlangen-Nürnberg in recognition of his achievements in metal physics fundamental research, in particular plasticity and fracture of metallic materials, 2005.

Prof. Dr.-Ing. A.R. Pyzalla was appointed Apl. Professor and Member of the Faculty of Mechanical Engineering of the Ruhr-Universität Bochum, May 2006.

Prof. Dr.-Ing. A.R. Pyzalla became associated member of the German committee "Komitee Forschung mit Neutronen (KFN)", January 2006.

Prof. Dr.-Ing. A.R. Pyzalla became member of the beam time review panel MA (Materials) of the European Synchrotron Radiation Facility (ESRF), Grenoble, France, and member of the beam time review panel of BESSY, Berlin, Germany in spring 2006.

Prof. Dr.-Ing. D. Raabe was ranked 1st place of the TOP-10 list of the most important scientists In Germany below the age of 45, Zeitschrift Bild der Wissenschaft, June 2005.

Prof. Dr.-Ing. D. Raabe's paper "Overview on the Lattice Boltzmann Method for Nano- and Microscale Fluid Dynamics in Materials Science and Engineering" is the most frequently downloaded research paper of the journal "Modelling and Simulation in Materials Science and Engineering", downloaded more than 2000 times since appearance.

B. Schaff won the 2nd Prize at the Metallographie-Tagung in Erlangen for her micrograph showing the coupled eutectic growth of W precipitates in a mono-crystalline NiAl matrix, September 2005.

Dipl.-Ing. C. Sachs was announced as winner of the TMS Champion H. Mathewson Award 2007 for the paper "Homogeneous Steel Infiltration".

Dipl.-Ing. C. Sachs, Dipl.-Biol. H. Fabritius and Prof. Dr.-Ing. D. Raabe received the Best Poster Award at the MRS Fall Meeting 2006 for the poster "Fracture Behavior and Shear Resistance of Lobster Cuticle".

Dipl.-Chem. A.J. Smith and Dr.rer.nat. A.W. Hassel received the Poster Award for the best elaboration "Studying and Applying Metallic Nanowires Obtained from Electrochemical Treatment of Directionally Solidified Eutectics", 6th International Symposium on Electrochemical Micro & Nanosystem Technologies, Bonn, Germany, August 2006.

Dipl.-Chem. A.J. Smith,Prof. Dr.rer.nat. M. Stratmann and Dr.rer.nat. A.W. Hassel received the Award for the 2nd best students talk "Studying Passive Materials under Erosion-Corrosion Conditions using Single Particle Impingement Experiments", 56rd Meeting of the International Society of Electrochemistry, Edinburgh, UK, August 2006.

Prof. Dr.rer.nat. M. Stratmann was elected full member of the North Rhine-Westphalian Academy of Sciences, Engineering and Economy Class, 2005.

Prof. Dr.rer.nat. M. Stratmann received the Willis Rodney Whitney Award 2005 of the NACE International (National Association of Corrosion Engineers) in recognition of his important contributions to corrosion science, Houston, April 2005.

Prof. Dr.rer.nat. M. Stratmann received the U.R. Evans Award, which is the top award of the British Institute of Corrosion, for his pioneering work in corrosion research on the occasion of the UK Corrosion 2005 conference in Manchester and was appointed honorary member of the British Institute of Corrosion for life, 2005.

Prof. Dr.rer.nat. M. Stratmann was elected member of the editorial board of "Journal of Solid State Electrochemistry" (2005).

Prof. Dr.rer.nat. M. Stratmann was elected Chairman of the Chemical-Physical-Technical Section of the Max-Planck-Society and became Member of the Senate of the Max-Planck-Society (2006).

M.Sc. T. Takahashi was awarded the Friedrich-Wilhelm Award of the RWTH Aachen (Rheinisch-Westfälische Technische Hochschule Aachen), December 2005.

Dr.-Ing. habil. M. Winning obtained a Heisenberg-Scholarship of the Deutsche Forschungsgemeinschaft, January 2006.

M.Sc. N. Zaafarani, Ph. D.R. Singh, Dr.-Ing. S. Zaefferer, Dr.rer.nat. F. Roters and Prof. Dr.-Ing. D. Raabe received the Best Poster Award for their contribution "3D experimental investigation and crystal plasticity FEM simulation of the texture and microstructure below a nanoindent in a Cu-single crystal" of the international committee of the 6th European Symposium on Nano-Mechanical Testing" (Nanomech 6), September 2005.

Dr.-Ing. S. Zaefferer received the ThyssenKrupp Werkstoff-Innovationspreis 2006, October 2006.

Participation in Research Programmes

National:

AVIF

Investigations on the high temperature corrosion of metallic materials under waste incineration conditions at temperatures of 300 - 600 °C

BMBF

Release systems for the self-healing of polymer/metal interfaces

Tailored adhesion mechanisms in composite systems by means of chemical surface functionalisation

Development and characterisation of high strength and supra ductile TRIP/TWIP light weight steels based on Fe-Mn-Al-Si

Adhesive properties of passive films on Zn-alloys

Characterization of microstructures and properties of ultra-high strength quasieutectoid Fe-C-Al steels containing higher carbon and aluminium contents (BMBF/BMWA)

DFG

Ab initio description of temperature dependent effects in dimensionally constrained magnetic shape memory Heusler alloys

Al-rich AlTi-alloys: Transformation of h-Al_2Ti and Al_5Ti_3 and formation of lamellar γ-TiAl + r-Al_2Ti microstructures

Development of ferritic iron-aluminium-tantalum alloys with strengthening Laves phase with highest creep strength in corrosive atmospheres

Effect of the scale effect of the tribological interface on the tribology of metal forming processes.

Grain boundary mechanics

Growth and simulations of quaternary GaInAsN quantum dots

Hardening of novel iron-chromium-aluminium-nickel alloys through coherent precipitates

Heat resistant super ferritic steels - Thermodynamic and kinetic calculations of precipitation reactions

High temperature corrosion by carburisation of Fe-Al alloys

High temperature materials

Improvement of the deformation properties of TRIP-, TWIP- and conventional steels by biaxial loading in compression and tension combined with additional torsion

Initial stages and kinetics of oxidation of binary and ternary iron-aluminides

Investigation of size effects with respect to texture and anisotropy

Investigations on mechanical properties and hot deformation behavior as well as microstructural characterization of Fe_3Al base alloys

Modeling of phase and microstructure formation under non-equilibrium conditions of Ti-Al laser welded seams

Nanofluid mechanics

Non-equilibrium flow at gradient surfaces: multi-component fluids

Oxidation and segregation on high strength steels

Physics of nitride-based, nanostructured, light-emitting devices

Production of nanowire arrays through directional solidificaton and their application

Project within the Schwerpunktprogramm SPP 1204 "Algorithmen zur schnellen, werkstoffgerechten Prozesskettengestaltung und -analyse in der Umformtechnik" WI 1917/5-1

Relationship between microstructure and damage mechanisms in multiphase steels

Simulation study on scaling effects in nano- and microscale fluid dynamics at deformable metal surfaces

Helmholtz Gemeinschaft

Virtual institute for photon and neutron research on advanced engineering materials (VI-PNAM)

Max Planck Society

Computational mechanics of polycrystals

The nature of Laves phases (Inter-institutional research initiative)

Triple-M: Multiscale materials modeling of condensed matter: Prediction of structures and phase diagrams in solid state chemistry

State of North Rhine-Westphalia

Ab initio description of iron and steel: Status and future challengers (ADIS 2006)

International Max Planck Research School (IMPRS) for surface and interface engineering in advanced Materials (SurMat)

Ag/TiO2-nanocomposite ultra-thin films (SurMat)

Fundamental Mechanisms of passivity break down of binary alloys (SurMat)

Intelligent self-healing by nano and micro-capsules (SurMat)

Microstructural aspects of passivity and corrosion of NiTi (SurMat)

Spatial screening of graded materials (SurMat)

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

Water at polymer/metal interfaces

European Science Foundation

Ab initio describtion of iron and steel: Status and future challengers (ADIS 2006)

EU

European network for surface engineering of new alloys for super high efficiency power generation

Interfacial phenomena at atomic resolution and multiscale properties of novel III-V semiconductors

Intermetallic materials processing in relation to earth and space solidification (IMPRESS)

Innovative demonstrations for the next generation of biomass and waste combustion plants for energy recovery and renewable electricity production (NextGenBiowaste)

Numerical modelling/lifetime prediction of delamination polymer coating disbonding and material degradation

RFCS (ECSC)

Advanced modelling of lateral flow and residual stresses during flat rolling

Characterisation of ultra-thin films on heterogeneous substrates

Development and evaluation of coatings and surface conditions on steel for antibacterial and easy to clean properties

Forming behaviour of corrosion protection primers

Fundamental aspects of corrosion and delamination behaviour of novel zinc alloy coatings and intermetallic Zn-phases

Fundamental aspects of conducting polymers for corrosion protection

High-strength long products with improved toughness and fatigue resistance

Induction assisted welding technologies in steel utilisation

Materials for increased performance in sustainable fuel combustion

New approaches in electrolytic cleaning of cold rolled steel sheets

Optimisation of in-service performance of boiler steels by modelling high temperature corrosion (OPTICORR)

Self-healing at cut-edge of coil-coated galvanized steel sheet

Simulation of barrier properties and formability of multilayer organic coatings

Tailored thin film plasma polymers for surface engineering of coil coated steel

Transformation behaviour of steel in the in-line hot rolling steel processing

Collaboration with Research Institutes and Industrial Partners

Research Institutes

National:

Access e.V., Aachen

Betriebsforschungsinstitut VDEh, Düsseldorf

BIAS, Bremen, Bremen

Clausthaler Umwelttechnik-Institut GmbH (CUTEC), Clausthal

Dechema Karl Winnacker Institut, Frankfurt/M.

Deutsches Elektronen-Synchrotron DESY, Hamburg

Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR): Institut für Raumsimulation, Köln

Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR): Zentrum für die Erstarrung unterkühlter Schmelzen (ZEUS), KölnForschungszentrum caesar, Bonn

Forschungszentrum Jülich GmbH: Institut für Werkstoffe und Verfahren der Energietechnik (IWV2), Jülich

Forschungszentrum Jülich GmbH, Jülich: Institut für Bio- und Nanosysteme (IBN-2), Jülich

Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung (IFAM), Bremen

Fraunhofer-Institut für Schicht- und Oberflächentechnik (IST), Braunschweig

Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Dresden

Fraunhofer-Institut für Werkzeugmaschinen und Umformtechnik, Dresden

Fritz Haber Institut der MPG, Berlin

Georg-August-Universität Göttingen, I. Physikalisches Institut, Göttingen

Gesellschaft zur Förderung der analytischen Wissenschaften e.V.: ISAS - Institute for Analytical Sciences, Dortmund

Gesellschaft zur Förderung der Spektrochemie und angewandten Spektroskopie (GFSAS) e.V., Dortmund

GKSS-Forschungszentrum Geestacht GmbH: Institut für Werkstoffforschung, Geesthacht

Gottfried-Wilhelm-Leibniz-Universität Hannover: Institut für Mikrotechnologie, Garbsen

Hahn-Meitner-Institut Berlin, Berlin

Heinrich-Heine-Universität Düsseldorf, Institut für Angewandte Physik, Düsseldorf

Hochschule Karlsruhe - Technik und Wirtschaft: Fachgebiet Informatik, Karlsruhe

Humboldt-Universitat zu Berlin, Berlin

Innovationsgesellschaft für fortgeschrittene Produktionssysteme in der Fahrzeugindustrie mbH, BerlinInstitut für Kristallzüchtung, Berlin-Adlershof, Bonn

Johannes-Gutenberg-Universität Mainz: Institute of Physics, Mainz

Laser-Zentrum Hannover e.V., Hannover

Leibnitz-Institut für Festkörper- und Werkstoffforschung Dresden e.V.: Institute for Metallic Materials, Dresden

Leibniz Institut für Festkörper- und Werkstoffforschung Dresden e.V. Institute for Solid State Research, Dresden

Max-Planck-Institut für chemische Physik fester Stoffe, Dresden

Max-Planck-Institut für Festkörperforschung, Stuttgart

Max-Planck-Institut für Kohlenforschung, Mühlheim

Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig

Max-Planck-Institut für Metallforschung, Stuttgart

Max-Planck-Institut für Mikrostrukturphysik, Halle,

Max-Planck-Institut für Polymerforschung, Mainz

Otto-von-Guericke Universität Magdeburg: Institut für Werkstoff- und Fügetechnik, Magdeburg

Rheinische Friedrich-Wilhelms-Universtität Bonn: Institute for Applied Mathematics, Bonn

Rheinische Friedrich-Wilhelms-Universtität Bonn: Institute for Numerical Simulation, Bonn

Ruhr-Universität Bochum: Institut für Werkstoffe, Bochum

Ruhr-Universität Bochum: Lehrstuhl für Angewandte Festkörperphysik, Bochum

RWTH Aachen: Giesserei-Institut, Aachen

RWTH Aachen: IEHK - Institut für Eisenhüttenkunde, Aachen

RWTH Aachen: IMM, Aachen

Schweisstechnische Lehr- und Versuchsanstalt Halle GmbH, Halle (Salle)Technische Universität Berlin: Institute for Materials Science and Technology - Metallic Materials -, Berlin

Technische Universität Braunschweig: Institut für Werkzeugmaschinen und Fertigungstechnik (IWF), Braunschweig

Technische Universität Chemnitz: Professur Werkstoffe des Maschinenbaus, Chemnitz

Technische Universität Clausthal: Institut für Werkstoffkunde und Werkstofftechnik, Clausthal

Technische Universität Darmstadt: Institut für Werkstoffkunde (IfW), Darmstadt

Technische Universität Dresden: Institut für Strukturphysik, Dresden

Technische Universität Dresden: Institut für Werkstoffwissenschaft, Dresden

Technische Universität München: Forschungs-Neutronenquelle Heinz Maier-Leibnitz, Garching

Universität Bremen, Bremen

Universität des Saarlands: Lehrstuhl für Prozessautomatisierung, Saarbrücken

Universität Dortmund: UDTM, Dortmund

Universität Duisburg-Essen: Analysis, Duisburg

Universität Duisburg-Essen: Physik - Experimentalphysik, Duisburg

Universität Duisburg-Essen: Theoretical Low-Temperature Physics, Duisburg

Universität Erlangen-Nürnberg: Institut für Werkstoffwissenschaften, Lehrstuhl für Werkstoffwissenschaften (Allgemeine Werkstoffeigenschaften), Erlangen

Universität Gesamthochschule Siegen, Siegen

Universität Hannover: Institut für Elektrothermische Prozesstechnik, Hannover

Universität Karlsruhe: Institut für Mikrostrukturtechnik, Eggenstein-Leopoldshafen

Universität Paderborn, Paderborn

Universität Stuttgart, Stuttgart

Universität Ulm: Abt. Werkstoffe der Elektrotechnik, Ulm

International:

Akademia Gorniczo-Hutnicza: Wydział Inżynierii Materiałowej i Ceramiki, Katedra Chemii Nieorganicznej, Krakow, Polen

Aristotle University of Thessaloniki, Thessaloniki, Greece

British Ceramic Research Ltd., Penkhull, U.K.

Centre de Mise en Forme des Matériaux (CEMEF), Sophia Antipolis, France

Centre De Recherches Métallurgiques ASBL, Liege, Belgium

Centre De Recherches Métallurgiques CRM, Brussels, Belgium

Centre National de la Recherche Scientifique, EPM-MADYLAM, Grenoble, France

Centre National de la Recherche Scientifique, Delegation Cote D'Azur, Valbonne, France

Centro de Estudios e Investigaciones Tecnicas de Gipuzcoa, San Sebastian, Spain

Centro Sviluppo Materiali S.p.A, Pomezia Terme (Roma), Italy

CIRIMAT, Toulouse, France

Consiglio Nazionale delle Ricerche, IENI Milano, Milan, Italy

Consejo Superior de Investigaciones Cientificas, Madrid, Spain

Consiglio Nazionale delle Ricerche, Roma, Italy

Danmarks Tekniske Universitet: Institut for Produktion og Ledelse, Kongens Lyngby, Denmark

Ecole Nationale Supérieure d'Ingenieurs de Caen et Centre de Recherche, Caen, France

Ecole Polytechnique Féderale de Lausanne: Institute of Materials, Lausanne, Switzerland

Foundation for Research and Technology, Heraklion, Greece

Fudan University, Shanghai, China

Fundacion ITMA, Llanera, Spain

Helsinki University of Technology: Materials Processing and Powder Metallurgy, Espoo, Finland

Inst. f. Physikalische Chemie der Universität Wien, Vienna, Austria

Institut de Recherches de la Sidérurgie Francaise, Mézières-les-Metz, France

Institut National Polytechnique de Lorraine, Lorraine, France

Institut National Polytechnique de Toulouse, Toulouse, France

Institute of Chemical Problems for Microelectronics, Moscow, Russia

Institute of Physics and Materials, Brno, Tchechia

Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Russia

Instituto de Soldadura e Qualidade, Oeiras, Portugal

Instituto Superior Tecnico IST, Lissabon, Portugal

Instytut Podstawowych Problemow Techniki PAN, Warszawa, Poland

Joint Research Centre, Petten, The Netherlands

Katholieke Universiteit Leuven: Departement Metaalkunde en toegepaste materiaalkunde, Leuven, Belgium

Korrosions och Metallforskningsinstitutet AB (KIMAB) (The Swedish Corrosion Institute (SCI) AB), Stockholm, Sweden

Kungliga Tekniska Högskolan: Department of Theoretical Chemistry, Stockholm, Sweden

Kungliga Tekniska Högskolan: Termodynamisk Modellering, Stockholm, Sweden

Kungliga Tekniska Högskolan: Avdelningen för Metallurgi/Institution för Materialvetenskap, Stockholm, Sweden

Laboratoire de Thermodynamique et Phisicochimie Métallurgiques, Grenoble, France

Magyar Tudomanyos akademia kemiai kutatokozpont, Budapest, Hungary

MEFOS - The foundation for Metallurgical Research, Lulea, Sweden,

MIT, Department of Aeronautics and Astronautics, Cambridge, USA

National University of Ireland: Computer Integrated Manufacturing Research Unit (CIMRU), Dublin, Ireland

Nederlandse Organisatie voor Toegepast Natuurwetenschappelijk Onderzoek, Apeldoorn, The Netherlands

Onderzoekscentrum voor Aanwending van Staal (OCAS) N.V., Zelzate, Belgium

Oxford University Department of Materials, London, U.K.

Research Institute for Solid State Physics and Optics, Budapest, Hungary

Saint Petersburg State University: Centre for Advanced Professional Education, Russia

SINTEF Energiforskning AS, Trondheim, Norway

Swedish Institute for Metals Research, Stockholm, Sweden

Technical Research Center of Finland, Espoo, Finland

Technische Universität Graz: Institut für Werkstoffkunde, Schweißtechnik und Spanlose Formgebungsverfahren, Graz, Austria

Tohoku University: Institute for Materials Research, Sendai, Japan

Ufa State Aviation Technical University: Institute of Advanced Materials, Ufa, Russia

Universidad Complutense de Madrid, Madrid, Spain

Universidad de Malaga UMAG, Malaga, Spain

Universidade de Aveiro: Departamento de Física, Aveiro, Portugal

Universidade de Aveiro: IEETA - Instituto de Engenharia Electrónica e Telemática de Aveiro, Portugal, Aveiro, Portugal

Universität Leoben: Lehrstuhl für Modellierung und Simulation metallurgischer Prozesse, Leoben, Austria

Université Blaise Pascal-Clermont II, Aubiere, France

Université de Rouen: Groupe de Physique des Matériaux, Rouen, France

Universiteit Leiden: LIC/Katalyse en oppervlaktechemie, Leids Instituut Chemisch Onderzoek, Leiden, The Netherlands

University of Birmingham: IRC in Materials Processing, Birmingham, U.K.

University of Cambridge, Cambridge, U.K.

University of Greenwich: Centre for Numerical Modelling and Process Analysis, London, U.K.

University of Leeds: Institute for Materials Research, Leeds, U.K.

University of Limerick, Limerick, Ireland

University of Liverpool, Liverpool, U.K.

University of Manchester Inst. of Science and Technology, London, U.K.

University of Science and Technology, Beijing, China

University of Wales Swansea: Materials Centre of Excellence, Swansea, U.K.

Ustav materialov a mechaniky strojov SAV, Bratislava, Slovakia

Vanderbilt University: Department of Electrical Engineering & Computer Science, Nashville, USA

Vrije Universiteit Brussel: Materials and Chemistry, Brussels, Belgium

Xiamen-University: State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen, China

Industrial Partners

National:

ALD Vacuum Technologies AG, Hanau

Audi AG, Ingolstadt

BASF AG, Ludwigshafen

BASF Coatings AG, Münster

Bayerische Motorenwerke AG, München

Benteler Automobil GmbH & Co.KG, Paderborn

Brose Fahrzeugteile GmbH & Co. KG, Coburg

CHEMETALL GmbH, Frankfurt/M.

Continental AG, Hannover

CORUS Aluminium Profiltechnik Bonn GmbH, Bonn

DaimlerChrysler AG, Stuttgart

DOC Dortmunder Oberflächencentrum GmbH, Dortmund

Edelstahlwerke Buderus AG, Wetzlar

Emitec GmbH, Hörselberg

Ford Forschungszentrum, Aachen

Frenzelit GmbH & Co. KG, Bad Berneck

GKS Gemeinschaftskraftwerk Schweinfurt GmbH, Schweinfurt

Groche & Tilgner, Kalletal

Henkel KGaA, Düsseldorf

Honda R & D Europe, Offenbach / Main

Houghton GmbH, Aachen

Hueck Engraving, Viersen

Hydro Aluminium Deutschland GmbH, Bonn

Infineon Technologies, Dresden

IQ evolution GmbH, Aachen/Düsseldorf

ISPAT GmbH, Duisburg

Krupp VDM GmbH, Altena

MK Metallfolien GmbH, Hagen

Niobium Products Company GmbH, Düsseldorf

Poli Film GmbH, Wipperfürth

Rasselstein GmbH, Andernach

Rheinkalk GmbH, Wülfrath

Rheinzink GmbH, Datteln

Robert Bosch GmbH, Stuttgart

Salzgitter Mannesmann Forschungsinstitut, Duisburg

Salzgitter Mannesmann Forschung GmbH, Salzgitter

Siemens AG Power Generation, Mülheim
SJM Co. Ltd., Ludwigshafen
Styria Federn GmbH, Düsseldorf
Thyssen Krupp VDM, Werdohl
ThyssenKrupp Electrical Steel GmbH, Gelsenkirchen
ThyssenKrupp Stahl AG, Duisburg
Titan-Aluminium-Feinguss GmbH, Bestwig
Vattenfall Europe AG, Berlin
VAW aluminium AG, Bonn
Volkswagen AG, Wolfsburg

International:

Aceralia Corporacion Siderurgica S.A., Basauri-Vizcaya, Spain
Acerinox SA, Madrid, Spain
Afval Energie Bedrijf, Amsterdam, The Netherlands
Arcelor Research S.A., Puteaux, France
Arcelor Research SA, Maizieres-les-Metz, France
ASM Brescia SPA, Brescia, Italy
AVR - Afvalverwerking Rijnmond, Rozenburg, The Netherlands
Bekaert, Zwevegem, Belgium
Böhler Edelstahl GmbH & CoKG, Kapfenberg, Austria
Bosch Rexroth B.V., Boxtel, The Netherlands
Calcom ESI SA, Lausanne, Schwitzerland
CNH Belgium N.V., Zedelgem, Belgium
Corus Technology B.V., IJmuiden, The Netherlands
Corus UK Ltd, Sheffield, U.K.
Corus UK Ltd., London, U.K.
Elsa, Elkraft, Denmark
European Space Agency ESA/ESTEC, Noordwijk, The Netherlands
Doncasters Group Ltd, Melbourne, U.K.
Fundacion INASMET, San Sebastian, Spain
Galvalange SARL, Dudelange, Luxemburg
Kema Nederland BV, Arnhem, The Netherlands
Keppel Seghers Belgium NW, Willebroek, Belgium
NPL Managment Ltd., Teddington, U.K.
Oy Hydrocell Ltd., Järvenpää, Finland
QinetiQ Nanomaterials Ltd., London, U.K.
Rautaruukki Oyj, Helsinki, Finland

Recherche Et Developpement Du Groupe Cockerill Sambre SCRL, Liege, Belgium

Rolls-Royce Plc., London, U.K.

Sidenor I+D, S.A., Basauri -Vizcaya, Spain

SSAB Tunnplat AB, Borlänge, Sweden

Surface specialities SA, Anderlecht, Belgium

SVUM a.s. Prague, Prag, Tchechia

Thomas Swan Scientific Equipment Ltd, Cambridge, U.K.

Top Analytica Ltd., Turku, Finland

Tratamientos Superficiales Iontech S.A., Guipuzcoa, Spain

Turbocoating S.p.A., Solignano-Fraz. Rubbiano (Parma), Italy

Tylite International Oy, Kulho, Finland

voest Alpine Stahl GmbH, Linz, Austria

Patents

Date of Issue	Description	Inventors
Jan. 20, 2005	Beta-Titanlegierung, Verfahrung zur Herstellung eines Warmwalzproduktes aus einer solchen Legierung und deren Verwendung DE Patent No. 103 29 899.1	Frommeyer, G., Prof. (20%) Sibum, H., Dr., Deutsche Titan GmbH (40%) Knippscheer, S., Dr. (20%) Schauerte, O., Dr., Volkswagen AG (20%)
June 13, 2005	Hochfester C-Stahl mit Superplastizität DE 10 2005 027 258.4	Frommeyer, G., Prof. Gerick, A., Dr., DaimlerChrysler AG Haug, T., Dr., DaimlerChrysler AG Kleinekathöfer, W., Dr., DaimlerChrysler AG

Date of Pending	Description	Inventors
Aug. 1, 2005	Verfahren zum Beschichten metallischer Oberflächen mit einer korrosionsschützenden Beschichtung EP 2005 008 309	Stratmann, M., Prof. Rohwerder, M., Dr. Paliwoda-Probeska, G. Chemetall GmbH TU Dresden
Aug. 1, 2005	Verfahren zum Schützen einer metallischen Oberfläche mit einer korrosionsinhibierenden Beschichtung EP 2005 008 306	Stratmann, M., Prof. Rohwerder, M., Dr. Paliwoda-Probeska, G. Chemetall GmbH TU Dresden
Aug. 3, 2005	Verfahren zum Beschichten von feinen Partikeln mit leitfähigen Polymeren EP 2005 008 314	Stratmann, M., Prof. Rohwerder, M., Dr. Paliwoda-Probeska, G. Chemetall GmbH TU Dresden
Dec. 2, 2005	TRIPLEX-Leichtbaustahl für Anwendungen im Fahrzeugbau DE 10 2005 057 599.4	Brüx, U., Dipl.-Phys. Kiese, J., Dr., Volkswagen AG Glatzer, M., Dipl.-Ing., Volkswagen AG
Dec. 23, 2005	Werkstoff für Bauteile einer Gasturbine DE 10 2005 0601 790.5	Sauthoff, G., Dr. Smarsly, W., Dr., MTU Aero Engines GmbH
Febr. 9, 2006	Kolben für Verbrennungsmotoren und Verfahren zur Herstellung eines Kolbens für Verbrennungsmotoren DE 10 2006 007 148.4	Frommeyer, G., Prof. Brüx, U., Dipl.-Phys. Walz, W., Dipl.-Ing., VW AG Kiese, J., Dr., VW AG

Conferences, Symposia, and Meetings Organized by the Institute

2005

F. Stein organized and chaired the Workshop The Nature of Laves Phases IV. Seven presentations were given at this international meeting held at the Max-Planck-Institut für Eisenforschung on Jan. 13, 2005.

M. Palm and F. Stein organized and chaired the symposium "(Inter-)Metallic High-Temperature Materials – Trends and Prospects" on the occasion of Dr. Gerhard Sauthoff's 65th birthday. About 80 participants attended the 5 invited talks by Prof. Dr. R.W. Cahn, University of Cambridge, Prof. Dr. D.G. Morris, CENIM, Madrid, Prof. Dr. M. Takeyama, Tokyo Institute of Technology, Prof. Dr. K.S. Kumar, Brown University, Providence and Prof. Dr. M. Heilmaier, Universität Magdeburg. The symposium was held at the Steel Institute VDEh, Düsseldorf, Jan. 14, 2005.

D. Raabe together with Prof. J. Urai and Prof. G. Gottstein (RWTH Aachen) organized the international workshop Computational Approaches in Materials Science, Mechanics, and Geosciences (GeoMat) with the support of the DFG where materials scientists, geoscientists, mechanicians and mathematicians from several continents met. The workshop was held at the Novotel in Aachen on June 8-10, 2005.

D. Raabe co-chaired (together with Prof. H. Fraser from Ohio State University and Prof. T. Pollock from Michigan State University) the 3rd International Breitnau Materials Conference Rapid Materials Maturation and Simulation which was organized jointly by the Max-Planck-Institut für Eisenforschung, US Air-Force, the Ohio-State University, and the Fraunhofer Institute for Mechanics of Materials IWM in Freiburg and was held in June 2005.

J. *Neugebauer* was publication chairman and member of the program committee of the 6th International Conference on Nitride Semiconductors (ICNS-6). The conference had more than 700 participants and more than 500 oral and poster presentations. ICNS-6 took place in Bremen on Aug. 8 - Sept. 2, 2005.

D. Raabe was a co-organizer of the 17th International Conference on Soft Magnetic Matter (SMM 17) which was held in Bratislava, Slovakia on Sept. 7 - 9, 2005.

F. Roters organized the 15th International Workshop on Computational Mechanics of Materials (IWCMM 15). It was attended by more than 90 participants from 9 countries. There were 32 oral contributions in two parallel session series, and 45 poster presentations. The workshop was held at the Max-Planck-Institut für Eisenforschung on Sept. 19 -20, 2005.

2006

J. Konrad, M. Palm, M. Spiegel and F. Stein organized and chaired the 3rd Discussion Meeting on the Development of Innovative Iron Aluminium Alloys - FeAl 2006. About 75 participants from 12 countries attended the meeting which comprised nine sessions with 56 contributions. It was held at the Treff Hansa Hotel, Mettmann, Germany, Jan. 22 - 24, 2006.

M. Friak, T. Hickel and J. Neugebauer organized and chaired the 1st conference on Ab initio Description of Iron and Steel (ADIS 2006) with 44 participants. The conference was held at Schloss Ringberg/Tegernsee on Febr. 19 - 24, 2006.

J. Neugebauer organized (together with J. Neuhaus (TU München) and S. Müller (Uni Erlangen)) and chaired the Symposium Materials Modelling at the joint meeting of the European Physical Society Division of Condensed Matter Physics and the Spring Meeting of the German Physical Society Condensed Matter

Division. 18 papers were presented to more than 150 participants from several countries. The conference was held in Dresden, March 27-31, 2006.

D. Raabe chaired the Symposium Computational Plasticity of the GAMM 2006 Conference (Gesellschaft für Mathematik und Mechanik) in Berlin on March 27 - 31, 2006.

D. Raabe co-chaired the 7th GLADD meeting of the GLADD Conference Series on Materials Science of the University of Delft, the University of Gent, the Katholieke Universiteit Leuven, RWTH Aachen und Max-Planck-Institut für Eisenforschung (together with Prof. L. Kestens, Prof. P. Van Houtte und Prof. G. Gottstein) in Leuven on April 15, 2006.

P. Eisenlohr organized the Joint Strategy-Workshop Materials of the Fraunhofer Society and the Max Planck Society which was held at the Steel Institute VDEh in Düsseldorf on April 24 - 25, 2006.

A. Ardehali and D. Ponge organized the 2. Warmumformtag (Hot-Metal-Forming Conference) with 130 attendees which was held at the Max-Planck-Institut für Eisenforschung in Düsseldorf on June 20, 2006.

A. W. Hassel and M. Stratmann organized the 6th International Symposium on Electrochemical Micro & Nanosystem Technologies which was held in Bonn on Aug. 22 - 25, 2006.

J. Gnauk organised the “stahl.net@mpie”, the 2nd colloquium of the MPIE alumni network with about 75 participants attending 5 invited talks by Dr. C.-D. Wuppermann, Steel Institute VDEh, Dr. M. Köhler, Sundwiger Messingwerke, Dr. M. Steinhorst, Dortmunder Oberflächen Centrum, Prof. A. Pyzalla and Prof. J. Neugebauer. The colloquium was held at the Steel Institute VDEh, Düsseldorf, Sept. 1, 2006.

M. Palm organized and chaired the intermetallics part at the joint meeting of the Fachausschüsse Titan and Intermetallische Phasen (technical committees “titanium” and “intermetallic phases”) of the DGM with 45 participants and 10 presentations at Schloss Oppurg, Oppurg/Thüringen, Sept. 9, 2006.

D. Raabe and S. Zaefferer organized the 8th GLADD Meeting of the GLADD Conference Series on Materials Science of the University of Delft, the University of Gent, the Katholieke Universiteit Leuven, RWTH Aachen und Max-Planck-Institut für Eisenforschung. The meeting was held at the Max-Planck-Institut für Eisenforschung on Sept. 29, 2006.

J. Neugebauer and O. Marquardt organized the 1. Harzer Ab Initio Workshop together with the Department of Applied Theoretical Physics, Technical University Clausthal. This 3 days seminar with 20 participants (TU Clausthal, Max-Planck-Institut für Eisenforschung, Düsseldorf) and 20 oral presentations was held at Pixhaier Mühle, Clausthal-Zellerfeld, Oct. 22 - 25, 2006.

F. Roters organized the meeting Modellierung mehrphasiger Werkstoffe of the Fachausschuss Computersimulation of the DGM. 10 papers were presented to about 30 participants from several countries. It was held at the May-Planck-Institut für Eisenforschung on Nov. 15, 2006.

Institute Colloquia and Invited Seminar Lectures

2005

Morris, D.G., CENIM, Madrid, Spain:
Studies of the high temperature behaviour of iron aluminides (01-14-2005, Colloquium)

Takeyama,M., Tokyo Institute of Technology, Japan:
Physical metallurgy and alloy design for advanced wrought high-temperature materials utilizing GCP and TCP compounds (01-14-2005, Colloquium)

Kumar, K.S., Brown University, Providence, USA:
Microstructure and mechanical properties of multiphase Mo-Si-B alloys (01-14-2005, Colloquium)

Heilmaier, M., Universität Magdeburg:
Industrial processing of high temperature structural intermetallics: current state and future trends (01-14-2005, Colloquium)

Faupel, F., Universität Kiel:
Polymer-Metal Nanocomposites for Functional Applications (02-10-2005)

Schneider, K., Leibniz-Institut für Polymerforschung Dresden:
Simultaneous Measurement of Local Strain and Structural Changes During Deformation and Failure of Polymer Materials (02-15-2005)

Bramfitt, B., International Steel Group Research, Bethlehem PA, USA:
Sinking of the RMS Titanic - A Metallurgical Perspective (02-21-2005)

Cerezo, A., Oxford University, UK:
Atomic-scale analysis of nanoscale engineering materials (02-22-2005, Colloquium)

Wegst, U. G.K., MPI für Metallforschung, Stuttgart:
Biological materials seen with the eyes of a material scientist — or from Ötzi to biomimetics (03-09-2005, Colloquium)

Larson, D. J., Imago Scientific Instruments, Madison WI, USA:
3-D Compositional Imaging at the Atomic Scale: Innovations in Atom Probe Technology (03-10-2005)

Speidel, M. O., ETH Zürich, Switzerland:
Austenitische rostfreie Stähle höchster Festigkeit UND Zähigkeit (03-17-2005)

Mücklich, F., Universität des Saarlandes, Saarbrücken:
Bio-inspired Structuring of Surfaces by Interfering Laser Beams (04-05-2005, Colloquium)

Horbach, J., Institut für Physik der Johannes-Gutenberg-Universität Mainz:
Influence of Chemical Short Range Order on Atomic Diffusion in Al-Ni Melts (04-14-2005)

Speer, J. G., Colorado School of Mines, Golden, Colorado, USA:
The “Quenching and Partitioning” Process - Background and Recent Progress (04-19-2005)

Spatz, J., MPI für Metallforschung, Stuttgart / Universität Heidelberg:
Biophysical Models of Cell Adhesion and Mechanics Applying Nano- and Microlithographic Tools (06-09-2005, Colloquium)

Bolmaro, R. E., Rosario National University, Argentina:
Regarding Microstructure Evolution at Large Deformations: Simulation Supported Analysis of Microstructures and Textures (07-04-2005)

Schneibel, J. H., Oak Ridge National Laboratory, USA:
Fabrication and Properties of Structural High-Temperature Mo-Si-B Alloys (07-05-2005, Colloquium)

Yoshimi, K., Tohoku University, Sendai, Japan:
Nano-Scaled Surface Self-Patterning in B2-type Intermetallics by Vacancy Engineering (07-08-2005)

Qteish, A., Yarmouk University, Jordan:
EXX and EXX based GW calculations of the electronic structure of semiconductors (08-04-2005)

Smith, A., Ohio University, Atlanta, USA:
Scanning Tunneling Microscopy Investigations of Transition Metal Nitride (08-09-2005)

Van de Walle, C., University of California, Santa Barbara, USA:
Hydrogen in Semiconductors, Oxides and Solutions (08-26-2005)

Entel, P., Universität Duisburg-Essen:
First-principles investigations of the instability leading to martensitic phase transformations (09-02-2005)

Sawada, K. and M. Yoshino, National Institute for Materials Science, Tsukuba,Japan:
Precipitation Behavior of Z phase during Aging and Creep in 9-12%Cr Ferritic Heat Resistant Steels; Precipitation Behaviour of MX Carbonitiride in High Cr Ferritic Steels (09-09-2005)

Neumann, W., Humboldt-Universität zu Berlin:
Interfacial Structures and Processes in Ni-based Superalloys (09-13-2005, Colloquium)

Petrov, M., Masaryk University, Brno, Czech Republic:
Molecular Dynamics of Amphiphiles (09-14-2005)

Marquardt, O., Humboldt-Universität zu Berlin:
Physik mit Links - a multimedia physics course (09-15-2005)

Dosch, H., MPI für Metallforschung, Stuttgart:
Premelting of Ice at Interfaces: A Nano-Phenomenon with Giga-Impact (10-11-2005, Colloquium

Miehe, C., Universität Stuttgart:
Variational-Based Multiscale Modeling of Inelastic Materials (10-17-2005

Richter, M., Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden:
Detection of Lifshitz transitions: a demanding task for both experiment and theory (10-18-2005)

Krack, M., Swiss Federal Institute of Technology, Zürich, Switzerland:
Fast and accurate density functional calculations experiment and theory (10-27-2005)

Pinto, H., TU Wien, Austria:
Characterization of Material and Component Deterioration using X-rays and Synchrotron Radiation (11-02-2005, Colloquium)

Nestler, B., Universität Karlsruhe:
Phase field modelling of grain structures and solidification processes (11-03-2005)

Albe, K., TU Darmstadt:
Atomistic computer simulations of metallic nanoparticles (11-08-05, Colloquium)

*Steinbach, I.,*ACCESS Research Center, Aachen:
The Multi Phase Field Method: Theory and Application (11-10-2005)

Krenke, T., Universität Duisburg-Essen:
Magnetische und strukturelle Eigenschaften von Ni-Mn-Sn und Ni-Mn-In Heusler-Legierungen (11-17-2005)

Neumann, K.-U., Loughborough University, Loughborough, U.K.:
Ni_2MnGa – Magnetic and Structural Properties (11-17-2005)

Emmerich, H., Institut für Gesteinshüttenkunde der RWTH Aachen:
Recent Problems in Phasefield Modelling (11-21-2005)

Schneider, M., Universität Augsburg:
Acoustically driven flow in microchannels and applications: From chaotic mixing to blood flow (11-21-2005)

Torizuka, S., National Institute for Materials Science, Sengen, Tsukuba, Ibaraki, Japan:
Creation of ultrafine-grained steel by high Z - large strain deformation: Bridging science and technology (12-12-2005)

Maier, J., MPI für Festkörperforschung, Stuttgart:
Electrochemical Function of Solids through Defects (12-13-2005, Colloquium)

Heine, V., University of Cambridge, U.K.:
The role of ab initio electronic structure calculations as “computer experiments”, with application to the energetics and effects of Ga impurities in Al grain boundaries (12-15-2005, Colloquium)

2006

Marx, D., Ruhr-Universität Bochum:
How do chemically bonded molecules detach from surfaces? (01-10-2006, Colloquium)

Kostka, A., University of Silesia, Katowice, Poland:
On the creep resistance of UFG microstructures formed by tempering of martensite and by ECAPing (01-11-2006)

Rinke, P., Fritz-Haber-Institut Berlin:
Combining quasiparticle energy calculations with exact-exchange density-functional theory (01-23-2006, Colloquium)

Asta, M., University of California, Davis, USA:
Nano-scale precipitation in Al-Sc and Fe-Cu alloys: Insights from first-principles calculations (02-01-2006, Colloquium)

Stierle, A., MPI für Metallforschung, Stuttgart:
Oxidation and Corrosion of Alloys on the Atomic Scale (02-02-2006)

Fleck, C., TU Berlin:
Bone and titanium alloys: Fatigue and corrosion behaviour of biomaterials (02-06-2006)

Kiessling, F.-M., IKZ Berlin:
Native and extrinsic defects in boron-reduced VCz GaAs crystals grown from Ga-rich melts (02-07-2006)

Rudolph, P., IKZ Berlin:
Dislocation cell structures in melt-grown semiconductor compound crystals (02-08-2006)

Uhlmann, P., Leibniz-Institut für Polymerforschung, Dresden:
Binary polymer brushes as a versatile tool to tune physico-chemical surface properties – application for studies of fluid flow and separation of liquids (02-23-2006)

Schmid, R., Ruhr-Universität Bochum:
A Car-Parrinello Molecular Dynamics Approach using Real Space (03-08-2006)

Gumbsch, P., IWM Freiburg:
Multiscale materials modelling - Bridging from atoms to the continuum (03-14-2006, Colloquium)

Vogel, S. C., Los Alamos National Laboratory, USA:
Capabilities for texture measurements of the new neutron diffractometer HIPPO (03-29-2006, Colloquium)

Lazo, C., TU Harburg:
A first-principles statistical mechanics study of the ordering behaviour of hydrogen on Pd (111) at low temperatures (04-03-2006)

Finnis, M., Imperial College London, U.K.:
Some theories of grain boundary embrittlement (04-04-2006, Colloquium)

Gaitzsch, U., IFW Dresden:
Martensite structures in NiMnG (04-26-2006)

Todorova, M., University of Sydney, Australia:
Order-disorder phase transitions: a DFT - (Wang-Landau) MC study (04-27-2006)

Isheim, D., Northwestern University, Evanston, Illinois, USA:
Development and microstructural characterization by 3-D atom probe microscopy of Cu-precipitation strengthened ferritic steels (05-02-2006, Colloquium)

Bieler, T. R., Michigan State University, East Lansing, MI, USA:
The Effect of Twinning and Crystal Orientation on Microcrack Initiation and Crack Propagation in Duplex TiAl Grain Boundaries (05-05-2006)

Baerthlein, S., Universität Erlangen-Nürnberg:
High-precision mixed-space cluster expansion for Cu-rich Cu-Pd alloys: Controlling the LPS group (05-10-2006)

Bieler, T. R., Michigan State University, East Lansing, MI, USA:
Microstructural evolution and heterogeneous deformation in lead-free solder joints due to thermomechanical cycling and creep (05-11-2006)

Evertz, T., Salzgitter Mannesmann Forschung GmbH, Salzgitter:
Modern Steels (05-17-2006)

Bieler, T. R., Michigan State University, East Lansing, MI, USA:
Development of deformation processing and welding strategies for ultra high purity niobium for future particle accelerators (05-19-2006)

Freysoldt, C., FHI Berlin:
Thin oxide films: analysis of finite-size effects (05-22-2006)

Al-Kassab, T., Universität Göttingen:
Atom probe tomography (APT): Recent achievements in the analysis of nano structures in metals (06-13-2006, Colloquium)

Wuttig, M., RWTH Aachen:
Theoretical and experimental investigations on shape change materials (06-14-2006)

Van de Walle, C., University of California, Santa Barbara, USA:
Defects and doping in Zn0 (06-21-2006)

Etou, M., Sumitomo Metal Industries Corporate R & D Labs, Ibaraki, Japan:
Development of super short interval multi-pass rolling technology for
ultra-fine-grained hot strip (06-23-2006)

Schön, C. G., Univ. São Paulo, Brasil:
Recent developments and challenges in computational materials modeling (07-11-2006, Colloquium)

Reuter, K., Fritz-Haber-Institut, Berlin:
First-principles statistical mechanics approaches to heterogeneous catalysis (07-17-2006, Colloquium)

Dupuis, A., ETH Zürich:
The dynamics of droplets on chemically and topologically patterned substrates (07-20-2006)

Behler, J. ETH Zürich, Switzerland:
Towards ab initio Metadynamics Simulations of Phase Transitions in Solids (08-01-2006)

Venkateswara Rao, M., MPI Stuttgart:
Application of ab initio calculations in thermodynamic modelling of phases (08-03-2006)

Kim, O., RWTH Aachen:
Thermodynamic optimization of the Al-Li phase diagram (08-14-2006)

Kioseoglou, J., Aristotle University of Thessaloniki, Greece:
Integrated methodology for the microstructural and energetical characterization
of interfacial defects: Partial dislocations in wurtzite GaN (08-22-2006)

Dluzewski, P., Polish Academy of Sciences, Warsaw, Poland:
Non-linear elasticity of nano-materials (08-29-2006)

Weber, S., Ruhr-Universität Bochum:
Development of sintered MMC with high wear resistance (08-31-2006, Colloquium)

Spitzer, K.-H., TU Clausthal:
Process and Materials Development: Examples of Experimental and Theoretical Investigations (09-15-2006, Colloquium)

Ramsteiner, I., Harvard DEAS, Cambridge, MA, USA:
High energy X-ray study of short range order and phase transformations in Ti-V (09-20-2006, Colloquium)

Uijttewaal, M., Radboud Universiteit Nijmegen, Netherlands:
Age old antipodes united: stable *and* low-work-function surfaces are generic (10-10-2006)

Hartley, C. S., El Arroyo Enterprises, Sedona, AZ, USA
Connection of Length Scales – The Key to Multiscale Modeling (10-11-2006)

Blügel, S., FZ Jülich:
Materials for Spintronic Devices by Computational Design (10-17-2006, Colloquium)

Strangwood, M., University of Birmingham, UK:
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Garcia, J., Boehlerit GmbH&Co.KG, Kapfenberg, Austria:
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Kadas, K., Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Budapest, Hungary:
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Zinkevich, M., Max-Planck-Institut für Metallforschung, Stuttgart:
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Schneider, G. A., TU Hamburg-Harburg:
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Hackbusch, W., MPI für Mathematik in den Naturwissenschaften, Leipzig:
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Schuhmann, W., Ruhr-Universität Bochum:
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Doll, K., Max-Planck-Institut für Metallforschung, Stuttgart:
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A. T. Blumenau, MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Simulation in Adhesion Science, WS 2005/2006.

G. Frommeyer, TU Clausthal: Phasen für den Einsatz bei mittleren und hohen Temperaturen, WS 2004/2005.

G. Frommeyer, TU Clausthal: Innovative Leichtbaustähle für die Verkehrstechnik, SS 2005.

G. Frommeyer, TU Clausthal: Leichtbauwerkstoffe auf der Basis intermetallischer Phasenlegierungen, WS 2005/2006.

G. Frommeyer, TU Clausthal: Hochfeste und supraduktile Leichtbaustähle, SS 2006.

G. Grundmeier, MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Surface analysis by means of spectroscopic and microscopic techniques, WS 2005/2006.

G. Grundmeier, Ruhr Universität Bochum / Fakultät für Maschinenbau (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Fundamentals of Adhesion, WS 2005/2006.

G. Grundmeier, M. Rohwerder, MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Lab course on surface spectroscopy and microscopy, WS 2005/2006.

A. W. Hassel, Heinrich-Heine Universität Düsseldorf: Einführung in die Nanotechnologie, SS 2005.

A. W. Hassel, MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Modern Coating Technologies, WS 2006/2007.

A. W. Hassel, MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Electron and Ion Transfer Reactions at Surfaces and Interfaces, WS 2005/2006.

T. Meier and A. T. Blumenau, Univ. Paderborn: Quantenmechanik II, WS 2005/2006.

M. Muhler, Ch. Wöll and M. Stratmann, Ruhr Universität Bochum / Fakultät für Maschinenbau: Mechanical properties of surface dominated materials, SS 2006.

J. Neugebauer, Univ. Paderborn: Elektrodynamik, Thermodynamik, Statistische Physik, WS 2004/2005, WS 2005/2006.

J. Neugebauer, Univ. Paderborn: Aktuelle Fragen der Theoretischen Physik, WS 2004/2005, WS 2005/2006.

J. Neugebauer, Univ. Paderborn: Multiskalensimulationen (Wahlpflichttheoretikum), WS 2004/2005, WS 2005/2006.

J. Neugebauer, Univ. Paderborn: Computational Material Science (Praktikum), WS 2004/2005, WS 2005/2006.

A. Pyzalla, TU Wien: Fügetechnik (joining), SS 2006.

A. Pyzalla, TU Wien: Betriebsfestigkeit (service strength, Seminar), SS 2006.

A. Pyzalla, TU Wien: Schadensanalyse (failure analyses), SS 2006.

D. Raabe, RWTH Aachen: The History of Materials, SS 2005, SS 2006.

D. Raabe: Lectures in the framework of the “Foreign Collaborator” program together with the IGERT initiative (Integrative Graduate Education and Research Traineeship Program), funded by the US-National Science Foundation NSF (the program is with Professor Surya Kalidindi (Drexel University, USA), Professor Brent L. Adams (Brigham Young University, USA), Professor Hamid Garmestani (Georgia Tech., USA), Christopher Schuh (MIT, USA), und Salvatore Torquato (Princeton University, USA)).

D. Raabe: Lectures within the International Max Planck Research School on Surface and Interface Engineering in Advanced Materials (SURMAT), Ruhr-Univ. Bochum, 21. and 22. Febr. 21 -22, 2005.

D. Raabe, RWTH Aachen: Metals in Mythology, The Names of the Metals and their Origin, Money and Metallurgy – a small History of the Money, WS 2004/2005.

D. Raabe, RWTH Aachen: Micromechanics of Materials, WS 2004/2005, WS 2005/2006, WS 2006/2007.

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M. Rohwerder, G. Grundmeier and M. Stratmann, Ruhr Universität Bochum / Fakultät für Maschinenbau, Korrosion der Metalle, SS 2006.

F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2005/2006.

M. Spiegel, RWTH Aachen: Korrosion keramischer Werkstoffe, WS 2004/2005, WS 2005/2006, SS 2006.

M. Spiegel: MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Thin oxide scales on metals: Fundamentals of oxidation and segregation processes to metal surfaces, WS 2005/2006.

D. Stöver, M. Stratmann, W. Theisen, M. Pohl and G. Eggeler, Ruhr-Universität Bochum / Fakultät für Maschinenbau: Werkstoffkundliche Exkursionen, SS 2006.

M. Stratmann, MPIE (International Max-Planck-Research-School for Surface and Interface Engineering in Advanced Materials): Introduction into physical chemistry of surfaces and interfaces – theoretical models for the description of surfaces, WS 2005/2006.

M. Winning, RWTH Aachen: Theoretische Metallkunde II, SS 2006.

S. Zaefferer, International Max Planck Research School on Surface and Interface Engineering in Advanced Materials (SURMAT), Ruhr-Univ. Bochum: Analytical Transmission and Scanning Electron Microscopy, March 3 - 4, 2005.

S. Zaefferer, TU Clausthal: Workshop on Crystallographic Textures - basic course: Orientation Microscopy in the SEM, Orientation Microscopy in the TEM, April 13, 2006.

Oral and Poster Presentations

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Al-Sawalmih, A., H. Fabritius, L. Raue, P. Romano,C. Sachs, S.-B. Yi and D. Raabe: Orientation and Crystallographic Texture of Calcite and Chitin in Lobster Shell. (Euromat 2005, 09-05 till 09-08, 2005, Prague, Czech Republic)

Al-Sawalmih, A., P. Romano, C. Sachs and D. Raabe: Structure and texture analysis of chitin-bio-nanocomposites using synchrotron radiation. (MRS Spring Meeting, 2005-03, San Francisco, USA)

Al-Sawalmih, A.: Orientation Relation between Calcite and Chitin in Crustacean Arthropods. (ANKA-Synchrotron, 05-02, 2005, Dortmund)

Ardehali Barani, A. and D. Ponge: Effect of Austenite Deformation on the Precipitation Behaviour of Si-Cr spring Steels During Tempering. (Solid-Solid Phase Transformations in Inorganic Materials 2005 (PTM 2005) 05-29 till 06-03, 2005, Phoenix, USA)

Ardehali Barani, A. and D. Ponge: Microtexture and tensile properties of tempered martensitic steel 55SiCr6. (Lecture at the workshop KUL-UGent-RWTH-MPIE, 2005-04-15 Leuven, Belgium)

Ardehali Barani, A. and D. Ponge: Morphology of Martensite Formed From Recrystallized or Work-Hardened Austenite. (Solid-Solid Phase Transformations in Inorganic Materials 2005 (PTM 2005), 05-29 till 06-03, 2005, Phoenix, USA)

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Ardehali Barani, A., D. Ponge and R. Kaspar: Improvement of Mechanical Properties of Spring Steels through Application of Thermomechanical Treatment. (Steels for Cars and Trucks, 06-05 till 06-10, 2005, Wiesbaden)

Ardehali Barani, A., L. Fei, P. Romano and D. Ponge: Effect of Vanadium and Thermomechanical Treatment on the Properties of 55SiCr6. (Super-High Strength Steels, 1st International Conference, 11-02 till 11-04, 2005, Rome, Italy)

Asteman, H. and M. Spiegel: Investigation of the chemical breakdown of protective oxides formed on pre-oxidized alloys caused by HCl (g) and H2O (g). (Eurocorr 2005, 2005-09-04 to 2005-09-08, Lisbon, Portugal).

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Bastos da Silva, A., S. Zaefferer and D. Raabe: Characterization of nanostructured electrodeposited NiCo Samples by use of Electron Backscatter Diffraction (EBSD). (MRS Spring Meeting, 03-28 till 04-01, 2005, San Francisco, USA)

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Hickel, T. and J. Neugebauer: Ab initio description of grain boundaries and diffusion processes. (Arbeitstreffen der Helmholtz-Allianz „HYPER“,, 2006-10-12 to 2006-10-13, Darmstadt).

Hickel, T. and J. Neugebauer: Ab initio Simulation von Grenzflächen. (Arbeitstreffen der Helmholtz-Allianz „Werkstoffübergänge“, 2006-06-13 to 2006-06-14, Geesthacht).

Hickel, T. and J. Neugebauer: Ab initio Thermodynamik und Kinetik. (Arbeitstreffen des SFB 761, 2006-09-28, Aachen).

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Hickel, T., B. Grabowski and J. Neugebauer: Ferromagnetic shape memory alloys: Thermodynamic and magnetic properites *(invited)*. (Joint group meeting at Material Research Laboratory of University of California, Santa Barbara, 2006-05-03, Santa Barbara, USA).

Hickel, T., B. Grabowski and J. Neugebauer: Temperature and magnetic field dependent properites of Ni2MnGa. (DPG Spring Meeting of the Division Condensed Matter, 2006-03-26 to 2006-03-31, Dresden).

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Kobayashi, S. and S. Zaefferer: Thermal Stability of Carbide Particles in Fe3Al-Cr-Mo-C Alloys. (3rd FeAl meeting, 2006-01, Düsseldorf)

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Marquardt, O.: An envelope potential approach to semiconductor quantum dots *(invited)*. (Inst. theor. Phys., 2006-03-06, Universität Bremen).

Marquardt, O.: Implementation and application of k*p calculations on InN/GaN nanostructures. (Solid-state physics seminar der Universität Bremen, 09-28-2006, Riezlern, Austria).

Marquardt, O.: Optical properties of quantum dots and wires (1. Harzer Ab initio workshop, Clausthal-Zellerfeld, 10-22 till 25, 2006).

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Neugebauer, J.: Ab-initio based multiscale growth simulations of group III-Nitrides *(invited).* (Parsem-Meeting, 02-13- till 02-15, 2006, Valbonne/France)

Neugebauer, J.: Materialdesign auf dem Computer *(invited).* (02-17-2006, IKZ, Berlin)

Neugebauer, J.: CVD Growth of Group-III Nitride Semiconductors: An ab Initio Based Multiscale Study *(invited).* (ECS-Meeting, 05-07 till 05-12, 2006, Denver/USA)

Neugebauer, J.: Ab-Initio Based Growth Simulations of Group-III-Nitrides *(invited)*, 05-02 till 05-07, 2006, UCSB Santa Barbara/USA

Neugebauer, J.: Ab initio calculations of free engergies and grain boundaries *(invited)*, 05-02 till 05-07, 2006, UCSB Santa Barbara/USA

Neugebauer, J.: Ab initio Beschreibung von thermodynamischen, kinetischen und mikrostrukturellen Mateiraleigenschaften: Status und zukünftige Herausforderungen *(invited)* (Kolloquium, 06-21-2006, TU Clausthal)

Neugebauer, J.: Ab initio multiscale simulation of materials *(invited)* (SFB-OTF Workshop, 07-24 till 07-26, 2006, Göttingen)

Neugebauer, J.: Ab initio Modellierung von Materialeigenschaften und –prozessen *(invited)* (Alumni-Meeting, 09-01-2006, MPIE Düsseldorf)

Neugebauer, J.: Modeling of crystal growth on atomistic scale *(invited)* (IWMCG5 Workshop, 09-10 till 09-13, 2006, Bamberg)

Neugebauer, J.: Bandgap issues and universal alignment of hydrogen levels in group-III nitride semiconductors *(invited)* (EW3NS-Workshop, 09-18 till 09-20, 2006, Kreta/Greece)

Neugebauer, J.: Extended Defects and Grain Boundaries in Al-based Materials *(invited)* (PSI-K COST-Workshop, 09-23 till 09-26, 2006, Wroclaw, Poland)

Neugebauer, J.: Obtaining thermodynamic and kinetic properties of surfaces from first principles *(invited)* (11-07-2006, Kolloquium, Universität Bochum)

Neugebauer, J.: Ab initio modellation of crystal growth *(invited)* (Polkom-Workshop, 11-13 to 11-17, 2006, Dresden)

Neugebauer, J.: Ab initio based materials design *(invited)* (IMPRS/Surmat-Workshop 12-06 till 12-08, 2006, MPIE Düsseldorf)

Nikolov, N., R. A. Lebensohn, F. Roters, D. Raabe and A. Ma: Micromechanical Modeling of Large Plastic Deformation in Semi-Crystalline Polymers. (Plasticity Conference 2006, 07-16 till 07-21, 2006, Halifax, Canada)

Nikolov, S., D. Raabe and F. Roters: A Constitutive Model for Glassy Polymers with Shear Transformation Zones Plasticity and Reptation-Based Viscoelasticity. (MMM Third International Conference Multiscale Materials Modeling, 09-18, 2006, Freiburg)

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Palm, M., A. Schneider and G. Sauthoff: Strengthening mechanisms for Fe-Al based alloys with increased creep resistance at high temperatures *(invited)*. (MRS Fall Meeting, 2006-11-27 to 2006-11-30, Boston, MS, USA).

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Petrov, M.: Theoretical elastic constants of α-chitin 1. Harzer Ab initio Workshop, Clausthal-Zellerfeld, 10-22 till 25, 2006)

Pinto, H. and A. Pyzalla: Internal stresses in Li2O-SiO2 glass-ceramics. (7th European Conference on Residual Stresses (ECRS 7), 2006-09-13 to 2006-09-15, Berlin, Germany).

Pinto, H., A. Pyzalla, H. Hackl and J. Bruckner: A comparative study of microstructure and residual stresses of CMT-, MIG- and laser-hybrid welds. (7th European Conference on Residual Stresses (ECRS 7), 2006-09-13 to 2006-09-15, Berlin, Germany).

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Pinto, H., A. Pyzalla, L. Ito, M. Crovace, E. B. Ferreira, F. Fauth, T. Wroblewski and E. D. Zanotto: Surface and Bulk Internal Stresses in Li2O-2SiO2 Glass Ceramics. (5th Annual Denver X-ray Conference, 2006-08-07 to 2006-08-11, Denver, USA).

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Ponge, D., A. A. Barani and D. Raabe: Thermomechanical treatment of spring steels. (International Conference on Advanced Steels, COM 2006, 10-02, Montreal, Quebec, Canada)

Ponge, D.: Modern high strength steels for automotive applications. (Conference 'Robust Processes with Modern Steels', INPRO Innovationsgesellschaft für fortgeschrittene Produktionssysteme in der Fahrzeugindustrie mbH, 06-08, 2006, Berlin)

Ponge, D.: Nanostrukturierte Stahlwerkstoffe – Eigenschaften, Analytik. (DVS-Forschungsseminar Nanotechnologie, 01-26, 2006, Materialprüfanstalt Universität Stuttgart

Ponge, D.: Warmumformbarkeit von Stahl. (Kontaktstudium Werkstofftechnik Stahl, Teil III, Technologische Eigenschaften, Institut für Umformtechnik und Umformmaschinen (IFUM), 08-28, 2006, Universität Hannover

Prymak, O., F. Stein, M. Palm, G. Frommeyer and D. Raabe: Konstitutionsuntersuchungen im System Nb-Cr-Al: Erste Ergebnisse und weitere Planungen. (Workshop: The Nature of Laves Phases VII, 2006-08-29, MPI für Metallforschung Stuttgart, Germany).

Pyzalla, A. R., H. Kaminski, B. Camin, W. Reimers, T. Buslaps and M. di Michiel: In-situ Synchrotron X-ray Studies of Creep Damage in CuZn-Alloys (*invited)*. (American Crystallography Association Meeting, 2006-07-22 to 2006-07-29, Honolulu, USA).

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Pyzalla, A. R.: Combined Diffraction and Tomography with white and monochromatic high energy synchrotron radiation (*invited)*. (ESRF User Meeting, 2006-02-07, ESRF Grenoble).

Pyzalla, A. R.: Materialforschung mit Neutronen und Synchrotronstrahlung (*invited)*. (Kolloquium des Instituts für Eisenhüttenkunde, 2006-06-12, RWTH Aachen).

Pyzalla, A. R.: Potential of space-resolved studies on materials with synchrotron radiation: crystalline texture of dinosaur bones (*invited)*. (Department für Geo- und Umweltwissenschaften, 2006-01-13, LMU München).

Pyzalla, A. R.: Synchrotronstrahlung zur Werkstoffcharakterisierung (*invited)*. (DGM-Tag 2006, 2006-06-08, Berlin, Germany).

Pyzalla, A. R.: Werkstoffcharakterisierung mit Synchrotronstrahlung (*invited)*. (Seminar des Instituts für Werkstofftechnik, 2006-07-03, TU Freiberg).

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Pyzalla, A.: Applications of Synchrotron Radiation, Neutrons and Ions in Engineering Material Science (*invited)*. (SNI 2006, German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities, 2006-10-04 to 2006-10-06, Hamburg).

Pyzalla, A.: Diffraktion und Tomographie zur Untersuchung von Ingenieurwerkstoffen (*invited)*. (ANKA, Industrieforum Kernforschungszentrum Karlsruhe, 2006-11-17, Karlsruhe).

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Raabe, D.: Crystal Mechanics and Fresh Lobster. (Gordon laboratory Invited Kolloquium Lecture 05-12, 2006, University of Cambridge, England)

Raabe, D.: Advances in Constitutive Modeling in Crystal Plasticity FEM. (Colloquium Lecture at the Department for Aeronautics at the Massachusetts Institute of Technology, 03-30, 2006, Cambridge, USA)

Raabe, D.: Crystal Mechanics and Fresh Lobster. (2006-05-12, Colloquium Lecture, University Cambridge)

Raabe, D.: Neues aus der Eisenzeit – Simulationen und Experimente in der Kristallmechanik und frischer Hummer. (Kolloquium an der Bundesantalt für Materialforschung (BAM), 08-22, 2006, Berlin)

Raabe, D.: Recent Advances in Crystal Mechanics and Chitin Composites. (Physics Colloquium at the Physics Department of the Technical University Dresden, 05-29, 2006, Dresden)

Rablbauer, R.: Ferritic Stainless Lightweight Fe-Al-Cr-Steels. (IOM MATERIALS CONGRESS 2006, 2006-04-05, London, UK).

Rasp, W. and A. Yusupov: Modelling of Spread and Side-Form Function in Hot Rolling by Different Upper-Bound Approaches. (III rd European Conference on Computational Mechanics (III rd ECCM), 2006, Lisboa, Portugal)

Rasp, W. and A. Yusupov: Upper-Bound Modelling of Lateral Flow in Hot Rolling. (9th International ESAFORM Conference on Material Forming, 2006, Glasgow, Scotland)

Rasp, W., C. M. Wichern and J. Valentin: Correlation of Surface Topography and Friction Coefficient for Different Metals Subjected to Flat Die Drawing. (25th Int. Deep-Drawing Research Group Congress (IDDRG), 2006 Porto, Portugal)

Rohwerder, M. and M. Stratmann: Delamination of Polymer/metal Interfaces: On the Role of Electron Transfer Reactions at the Buried Interface. (209th Meeting - X1 - Electron Transfer Reactions at Organic/Metal Interfaces: From Molecular Monolayer Modified Electrodes to Buried Polymer Metal Interfaces, 2006-05-07 to 2006-05-12, Denver, Colorado, USA).

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Rohwerder, M.: Conducting polymer containing nanocomposite films for smart corrosion protection. (Chemical Nanotalks (CNT) VII, 2006-10-23 to 2006-10-25, Frankfurt).

Rohwerder, M.: High Resolution Kelvin Probe Microscopy: Scanning Kelvin Probe Force Microscopy (SKPFM) vs. classical Scanning Kelvin Probe (SKP). (EMNT 2006, 6th INTERNATIONAL SYMPOSIUM ON ELECTROCHEMICAL MICRO& NANOSYSTEM TECHNOLOGY, 2006-08-22 to 2006-08-25, Bonn).

Rohwerder, M.: Intelligent Corrosion Protection by Conducting Polymers *(invited)*. (Smart Coatings 2006, 2006-02-15 to 2006-02-17, Orlando, USA).

Rohwerder, M.: Intelligenter Korrosionsschutz mittels Nanocomposite Coatings auf Basis leitfähiger Polymere *(invited)*. (Polymers & Coatings 2006, 2006-09-24 to 2006-09-26, Universität Mainz, Mainz).

Romano P., H. Fabritius, C. Sachs *and D. Raabe*: Lobster Cuticle as an Example of Smart Anisotropic Material. (2006 TMS Annual Meeting & Exhibition, Symposium: Biological Materials Science Session: Biological Materials, 03-12 till 03-16, 2006, San Antonio, Texas, USA)

Romano, P., A. Barani, D. Ponge and D. Raabe: Design of High-Strength Steels by microalloying and thermomechanical treatment. (2006 TMS, 03-12 till 03-16, 2006, San Antonio, Texas, USA).

Roters, F. and Raabe, D.: Mechanism-oriented steel development. (New Methods of Steel Design, invited, 2006-06-30 Aachen)

Roters, F., A. Ma, N. Zaafarani and D. Raabe: Crystal plasticity FEM modeling at large scales and at small scales. (GAMM annual meeting, 03-27 till 03-31, 2006, Berlin)

Roters, F.: A Dislocation Density Based Constitutive Law for BCC Materials in Crystal Plasticity FEM. (THERMEC 2006, 07-04 till 07-08, Vancouver, Canada)

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Roters, F.: Mapping the crystal orientation distribution function to discrete orientations in crystal plasticity finite element forming simulations of bulk materials. (International Conference on Aluminium Alloys ICAA10, 2006-07 Vancouver, Canada)

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Habilitation, Doctoral, Diploma, Master, and Bachelor Theses

Habilitation Thesis

Dr.-Ing. habil. Grundmeier, G.: Interface Analysis and Engineering of Thin Functional Films on Metals. Ruhr-Universität Bochum (2006)

Doctoral Theses

2004 (residual since Scientific Report 2003/2004)

Dr.-Ing. Baumert, B.: Untersuchungen zum Schädlingsverhalten von ultra-dünnen Plasma-Polymer-Beschichtungen auf mechanisch belasteten Metallsubstraten. Ruhr-Universität, Bochum (2004)

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Dr.-Ing. Lücken, H.: Mikrotexturen innerhalb plastisch verformter Körner. RWTH Aachen(2005)

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Hantcherli, L.: Implementation of a particle pinning model in a cellular automaton based simulation of primary static recrystallization. RWTH Aachen, Ecole Nationale Supérieure des Mines de Saint-Etienne, France (2004)

Zambaldi, C.: Modellierung und experimentelle Untersuchung des Rekristallisationsverhaltens der Nickelbasis-Superlegierung CMSX-4. Univ. Regensburg (2004)

2005

Bubnik, V.: Interactive 3D-visualization of electronic charge densities. Brno University of Technology, Czech Republic (2005)

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Ramesh, M.: Experimental Investigation on Deformation Behaviour of Aluminium Oligocrystals. MIT Cambridge (USA), RWTH Aachen (2006)

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2006

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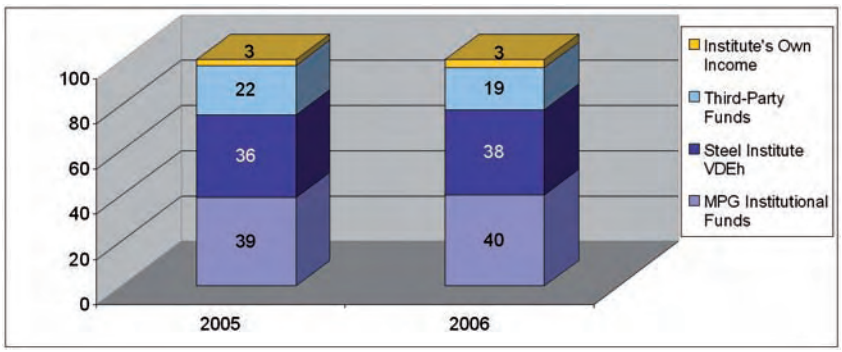
Budget of the Institute

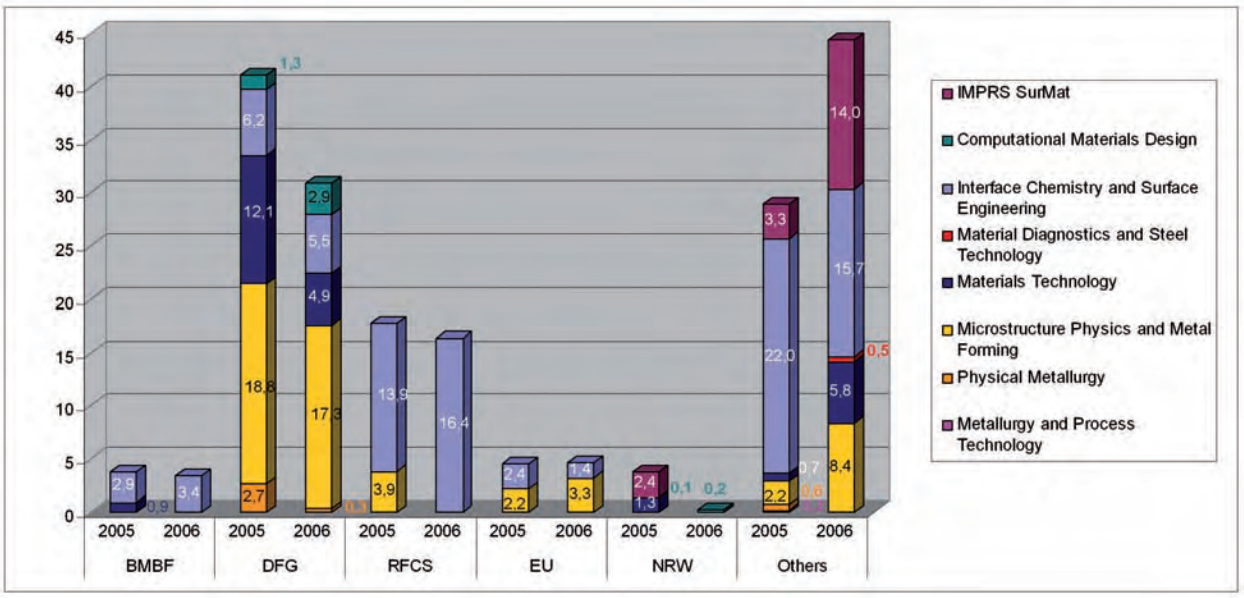
Revenue

(percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2006 data estimated)



Third-Party Funds

(percentual contributions to total revenue including personnel, material, investments; year 2006 data estimated))

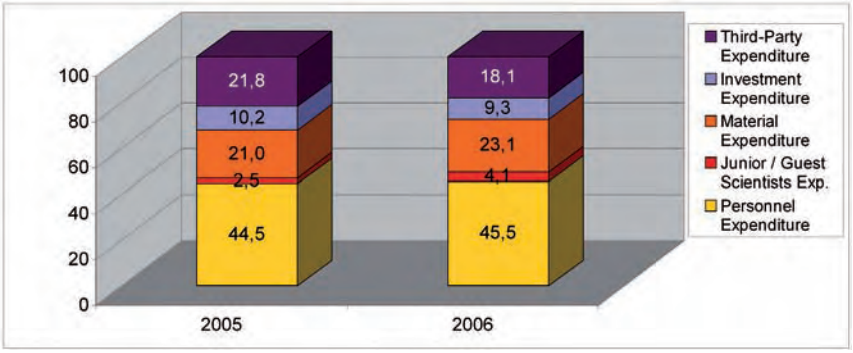


BMBF: Ministry of Science and Education
DFG: German Science Foundation
RFCS: Research Fund for Coal and Steel
(European Coal and Steel Community - ECSC)

EU: European Community
NRW: North Rhine-Westphalia

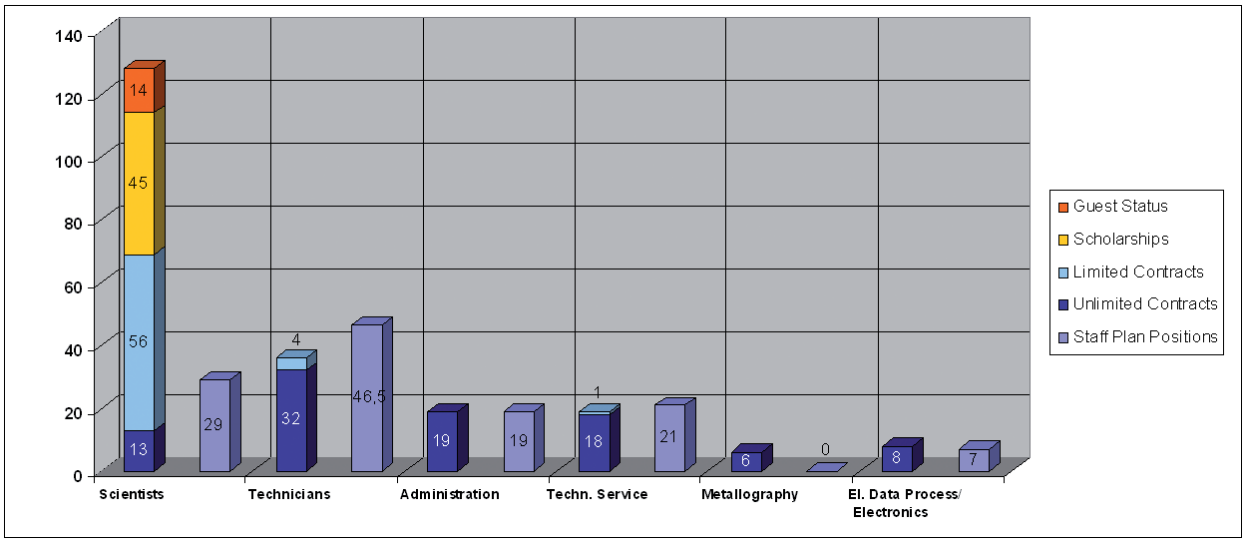
Expenditure

(percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2006 data estimated)

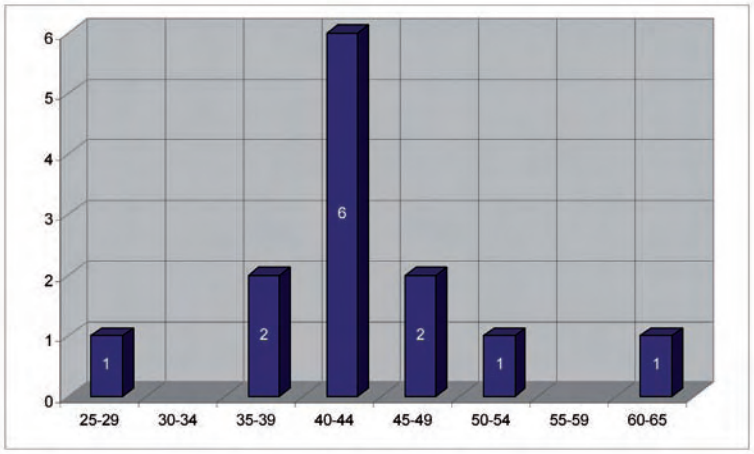


Personnel Structure

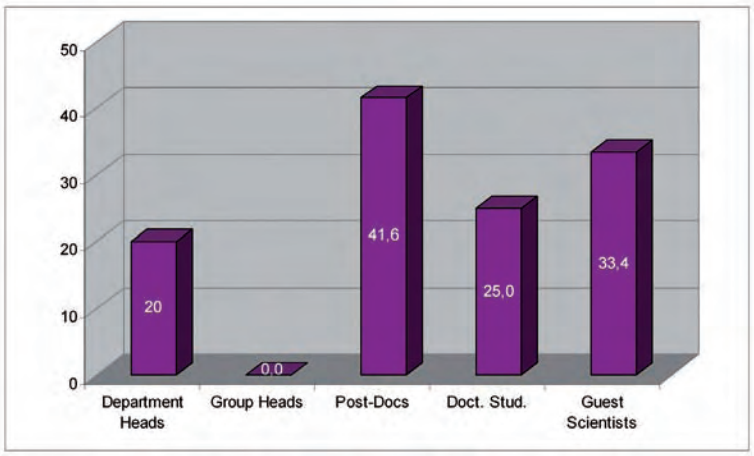
Number of Scientific / Non-Scientific Employees (Dec. 2006, estimated)



Age Distribution: Number of Scientists with Unlimited Contracts (Dec. 2006, estimated)
(total number: 13)

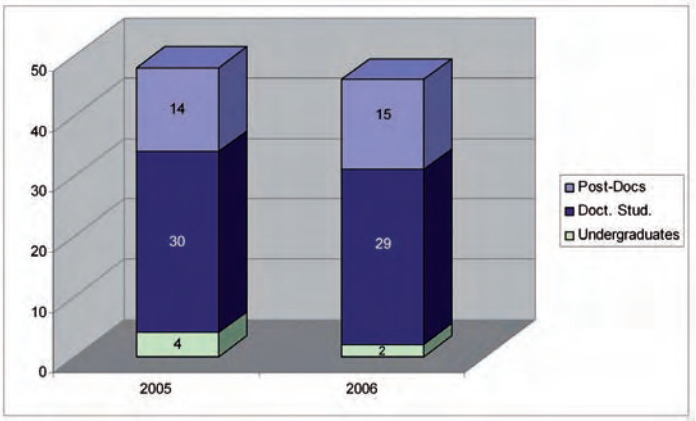


Female Scientists (Dec. 2006, estimated)
(percentual numbers)



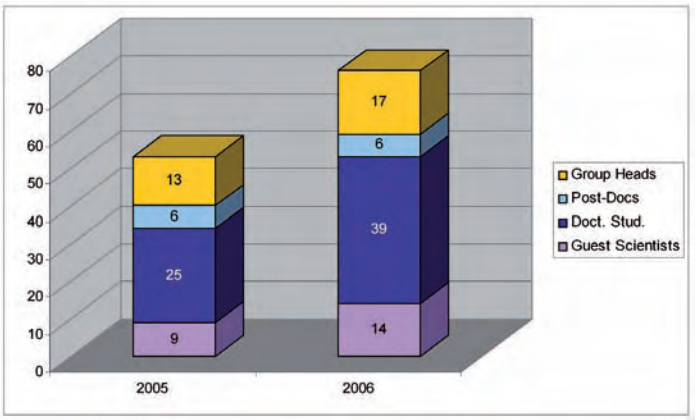
Number of Junior Scientists Financed via Third-Party Funds

(year 2006 data estimated)



Number of Junior Scientists not Financed via Third-Party Funds

(year 2006 data estimated)



The Institute in Public

Grammar school (Gymnasium) students from the Düsseldorf area visited the labs of the Max-Planck-Institut für Eisenforschung on Sept. 27, 2006 on the occasion of the Stahlcampus day of the Steel Institute VDEh with about 500 participants.

The institute joined the annual German Girls' Day action and opened its labs for girl students of the 5th girls' day on April 28, 2005. Also the North Rhine-Westphalian Minister of Schools, Youth and Children Ute Schäfer visited the institute on this occasion.

The North Rhine-Westphalian Minister of Innovation, Science, Research and Technologies Prof. Dr. rer. pol. Andreas Pinkwart visited the institute on Jan. 30, 2006 and was impressed by the multitude of innovations which were made possible by using the seemingly old material steel.

Prof. Dr. rer. nat. M. Stratmann addressed the role of extra-university research in innovation at a discussion meeting on the "NRW.Bank.Ideenschiff" ("North Rhine-Westphalian ship of ideas") on Sept. 6, 2006 which was part of an innovation initiative of the North Rhine-Westphalian Minister of Innovation, Science, Research and Technologies Prof. Dr. rer. pol. Andreas Pinkwart.

Dr. A. W. Hassel provided the cover photographs of the Brochure of the Ministry of Innovation, Science, Research and Technology of the state North Rhine-Westphalia and of the calendar „Bilder aus der Wissenschaft 2007" of the Max Planck Society.

The institute together with the Steel Institute VDEh again contributed to the annual German Tag der Technik (technology day) on June 17 - 18, 2005 and May 19 - 20, 2006 with the topic "Blick in den Stahl" (Looking into steel).

The Steel Information Centre produced a DVD entitled "Stahl - vom Eisenerz zum Hightech-Product" (Steel - From iron ore to high-tech products) with an interview by Dr. J. Gnauk on the occasion of the MPIE Alumni Meeting on Sept. 1, 2006 in the Steel Institute VDEh.

The International Workshop on "Ab initio Description of Iron and Steel Status and Future Challenges" (ADIS 2006) on February 19 - 24, 2006 organized by the Department of Computational Materials Design in the Ringberg Castle/ Bavaria was subject of the Ψ_k Newsletter: Ab initio (from electronic structure) calculation of complex processes in materials. No. 75, June 2006.

Repeatedly newspapers and journals reported on the work in the Max-Planck-Institut für Eisenforschung:

2005

Nov. 17, 2005	Rheinische Post	‚Spitzenforschung in Düsseldorf'
Nov. 24, 2005	Göttinger Tageblatt	‚Fehler machen den Stoff interessant'
02/2005	Stahl-Informations-Zentrum Nr. 9 als Beilage in: mobil - Das Magazin der Bahn Nr. 12	‚Ausgekocht'
06/2005	Bild der Wissenschaft	‚Der Überflieger'
06/2005	Konstruktion	‚Spitzenplatz bei den metallischen Werkstoffen: Stahl - ein universeller Struktur- und Funktionswerkstoff'
Oct. 3, 2005	Westdeutsche Allgemeine Zeitung (WAZ)	‚Professor weltweit gefragt: Erfindung ist Gold wert'
11/2005	FhG Research News	'Metals under the microscope'

2006

Jan. 10, 2006	Rheinische Post	‚Elfenbeintürme eher selten'
5/2006	Technology Review	‚Zeitreise im Dinoknochen'
6/2006	Stahl und Eisen 126 (2006) Nr. 1	‚Dem Stahl auf seinen kristallinen Grund gehen'

6/2006	Stahl und Eisen 126 (2006 Nr. 2	NRW – Wissenschaftsminister besucht MPIE
6/2006	Stahl und Eisen 126 (2006) Nr. 6	Stahl-Innovations-Preis
6/2006	Die Welt	Stahl-Innovations-Preis ‚Wunderwelt aus Blech'
3/2006	bayern Metall	‚Metalle unter der Lupe'
6/2006	Süddeutsche Zeitung	Gewinner des Stahl-Innovations-Preises
6/2006	Beilage SZ	‚Wunderwerk aus Blech'
6/2006	Informationen Stahlzentrum	Stahl-Innovationspreis
June 23, 2006	Süddeutsche Zeitung Wirtschaftsbeilage	‚Mit vereinten Kräften' Düsseldorfer MPI arbeitet mit der Industrie
June 25, 2006	NZZ am Sonntag Beilage ‚Wissen'	‚Karosserie aus dem Computer'
7/2006	stahl und eisen 126 (2006) Nr. 7, p. 134-146	, Atom für Atom zu neuen Werkstoffen'
8/2006	Advanced Engineering Materials 8 No.8, p. 2	‚Neue Stahllegierungen für den Automobilbau'
9/2006	Steel Research international 77 (2006) 9-10	'Steels for Automotive Applications'
9/2006	Steel Research international 77 (2006) 9-10, p. 760	'Prof. Pyzalla and Prof. Neugebauer New Directors at Max-Planck-Institut für Eisenforschung'
July 24, 2006	Der Spiegel (30/2006)	‚Materialforschung – Heißer Stahl aus Düsseldorf'
Aug. 3, 2006	Die Welt	‚Neue Stahllegierungen für den Automobilbau'
Aug. 18, 2006	Süddeutsche Zeitung	‚Absage an den Elfenbeinturm'
Sept. 29, 2006	Financial Times Deutschland Beilage "Stahlmarkt"	‚Ein Lächeln in einer Welt aus Stahl'
Oct. 14, 2006	Neue Ruhr/Neue Rhein Zeitung	‚Physik im Niemandsland'
11/2006	Faszination Stahl Nr. 11, p. 12	‚Heiße Eisen und kühle Rechner'
Nov. 13, 2006	MITTELSTAND, das Unternehmermagazin im Handelsblatt	‚Starke Federn brauchen einen guten Draht'

Likewise German broadcasting and TV reported on the institute:

March 11, 2005	3sat	tips&trends
March 12, 2005	3sat	Automobilsalon: ‚Faszination Stahl'
Aug. 15, 2005	WDR Fernsehen	Quarks & Co: ‚Stahl – kein altes Eisen'
Aug. 16, 2005	WDR Fernsehen	Quarks & Co: ‚Stahl – kein altes Eisen'
Aug. 28, 2005	Deutschlandfunk	Wissenschaft im Brennpunkt: ‚Weich wie Stahl'
Sept. 02, 2005	Deutsche Welle TV	Projekt Zukunft: ‚Stahl nach Maß'
Oct. 04, 2005	WDR Fernsehen	Quarks & Co: ‚Stahl – kein altes Eisen'
Aug. 23, 2006	WDR Fernsehen	TV trailer nanotechnology on the conference EMNT2006 in Bonn