RUHR-UNIVERSITÄT BOCHUM

RUB

Materials Research Department

No. 7 | 2010

news

Research Insights and Information

DEAR READER,

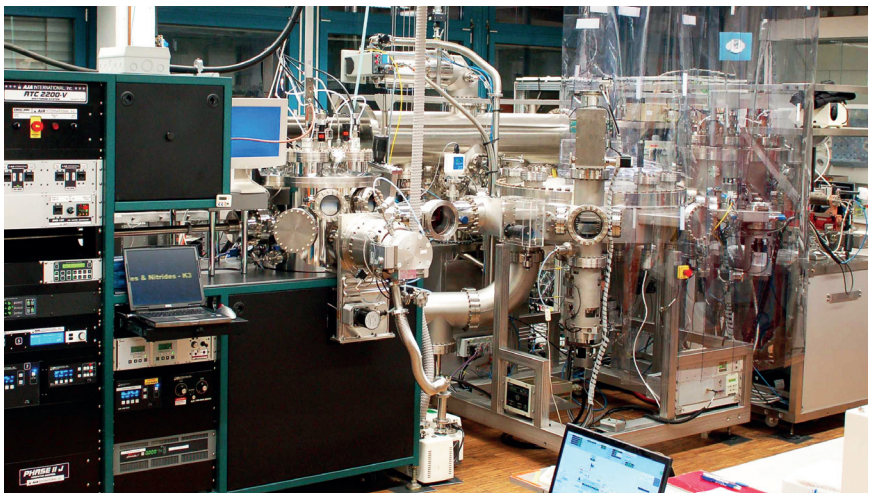
this first newsletter from our new *Materials Research Department (MRD)* (see article by G. Eggeler and U. Kunze) carries the No. 7, since it continues the tradition of our previous newsletter series "Materialwissenschaften" of the "Materialforum", to inform about fascinating research projects and current developments in "Materials Science and Engineering", one of the research strengths at the Ruhr-Universiät Bochum (RUB).

Due to the importance of the research area "Materials Science and Engineering" and the success of RUB researchers in applying for collaborative projects, the *"Research Department Integrity of Small-Scale Systems (IS³) / High-Temperature Materials (HTM)"* came into existence in 2009, which now has evolved into the Materials Research Department. It has transformed from a project platform where the focus lay on top-level *interdisciplinary research* projects, to an infrastructural element of the RUB, supporting the activities of materials scientists. The MRD is the interdisciplinary platform where materials scientists of RUB (from faculties of mechanical engineering, electrical engineering, chemistry, physics, mathematics and geosciences) as well as of surrounding research institutes (MPI-Eisenforschung Düsseldorf, MPI-Kohlenforschung Mülheim, DLR Köln, FZ Jülich) meet, discuss and advance research. Our pre-proposal "Combinatorial Materials Engineering" (CME) for a Cluster of Excellence in the Excellence Initiative evolved from the MRD platform.

In this issue of the newsletter, the recent history of materials science at RUB is briefly reviewed, basic concepts of the CME proposal are outlined, the new Center for Electrochemical Sciences and SFB-TR 87 are introduced, the continuation of IMPRS-SurMat is discussed, a scientific contribution treats materials for harsh environments, and ICAMS reports on recent developments. Finally, a new section of short news is added.

Yours sincerely,

Prof. Dr.-Ing. Alfred Ludwig



Research facilities (sputter deposition system) for combinatorial materials science

From "Materialforum" to the Materials Research Department

When the authors of this article joined the Ruhr-Universität Bochum (RUB) fifteen years ago, we could take over established materials science research groups focussing on microstructure and mechanical properties and magnetic and electric properties, respectively. Our start up activities in research and teaching were well supported, and before long we could pursue our research fields on a high level. But materials research at RUB at that time was heterogeneous and activities were spread over several faculties with only a little interaction. Shortly after we had arrived at RUB, our state North Rhine-Westphalia (NRW) made an effort to structure its university-based materials research activities, and Prof. Peter Scheid, Prorector for Research at the time, used this occasion to suggest a sharpening of our materials research profile. He suggested a closer collaboration between the individual materials groups and highlighted the benefits arising from a closer cooperation between all materials researchers.

We took up his suggestions and initiated the Materialforum of RUB, which started out with regular meetings of colleagues from mechanical and electrical engineering, physics, chemistry and geo-sciences. In the beginning four areas of expertise were identified as (i) microstructures and mechanical properties, (ii) nanostructured electronic materials, (iii) thin films and surface physics, and (iv) surface chemistry. The spokesmen of these four areas were G. Eggeler, U. Kunze, H. Zabel and M. Muhler. In the summer of 1997 we organized the first Materials Day at RUB with oral and poster contributions from all material disciplines, and we published a first circular with materials news from the RUB. The first Materials Day was very successful and the Materialforum soon evolved into a platform for exchange of scientific ideas as well as for effective shared use of expensive research equipment. But most importantly, a number of highly successful research activities emerged from the Materialforum, including collaborative research centers funded by the German Research Foundation (DFG): SFB 459 (shape memory technology), SFB 491 (magnetic hetero structures), SFB 526 (rheology of the earth) and SFB 558 (heterogeneous

catalysis). Moreover we were able to establish an interdisciplinary centre for Nano Structures and Nano Materials (funded by NRW). Together with the two Max Planck Institutes for Eisenforschung (MPIE, Düsseldorf) and Kohlenforschung (MPIK, Mülheim) we established an International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS SurMat).

In the summer of 2006 the Materialforum of RUB submitted a pre-proposal for the establishment of an Excellence Cluster in the framework of the German Excellence Initiative, with the title "Integrity of Small-Scale Systems". While this pre-proposal was finally not successful, it received still very positive resonance, such that its key ideas could be used to obtain funding to further strengthen cutting-edge materials research at RUB. As an important measure the interdisciplinary Materials Research Department (MRD) was founded (Director: A. Ludwig) with funding for 11 materials research projects which have the potential to act as nuclei for new initiatives. In parallel, RUB was successful in establishing a new research institute, the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), with three professors who work on scale bridging modelling approaches in materials science. Most recently the new SFB-TR 87 (plasma synthesis of nanostructured functional layers, Director: P. Awakowicz) was established.

Today, materials science and engineering is one of the declared research strengths of the RUB linking research activities from engineering and science departments. The materials researchers of RUB have decided to continue the activities of the original and successful Materialforum in today's Materials Research Department, with clearly defined objectives and best-practice rules for promotion of young researchers, gender equality and for identifying and strengthening promising materials research fields which are related to the four grand challenges of mankind: energy, health, environment and transport. We are glad to see the high interest which the 7th Materials Day at RUB receives, and that the tradition of informing the public by regular circulars is maintained. We wish A. Ludwig, our first director of the new Materials Research Department of the RUB success and we will support him in his endeavour to continue excellence in materials research at our university.

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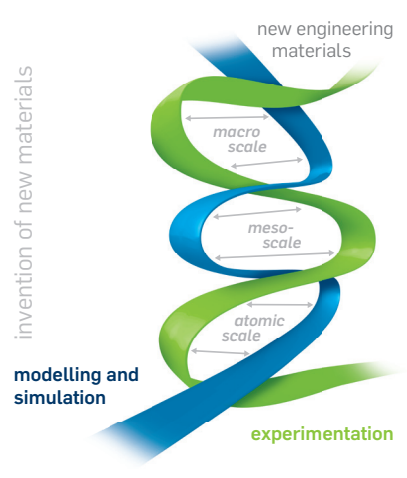
Combinatorial Materials Engineering (CME) –

Invention of New Engineering Materials by Scale Bridging Experimentation and Modelling

In the last round of the German Excellence Initiative, the material scientists of Ruhr-Universität Bochum (RUB) proposed an Excellence Cluster in the area of Materials Science and Engineering with the title *Integrity of Small-Scale Systems (IS³): Interface-Dominated Functional and Structural Material Properties*. The proposal received a positive scientific review. The research field of materials science at RUB has been significantly strengthened since 2006, when RUB material researchers made a first attempt to establish a Cluster of Excellence in Materials Engineering. Most importantly, the new research institute ICAMS for scale bridging materials modelling on all length scales was established, well-defined collaboration procedures between RUB and its external partners in materials research (Max Planck Institute für Kohlenforschung in Mülheim/Ruhr and Eisenforschung in Düsseldorf, DLR Cologne and FZ Jülich) were agreed upon, and the new Materials Research Department (MRD) was established, with the mission to act as an interdisciplinary platform for promoting excellence in materials research at RUB. Materials scientists at RUB cover a wide field of topics, ranging from atomistic simulations to failure analysis of engineering components. Therefore it was by no means easy to agree on a competitive research topic which best represents all strong elements of our materials research portfolio. For example, the topic *Science and Engineering of Materials for Energy Systems of the Future (SEMES)* was discussed for quite some time. But after intense discussions, we decided to go into another new direction. Our pre-proposal for an Excellence Cluster in the present round of the German Excellence Initiative is entitled: *Combinatorial Materials Engineering (CME) – Invention of New Engineering Materials by Scale Bridging Experimentation and Modelling*.

In *CME*, materials scientists from RUB reinforced by scientists from Max Planck Institutes (MPI Eisenforschung, MPI Kohlenforschung) and Helmholtz Centres (FZ Jülich, DLR Cologne, HZB Berlin) join forces. *CME* represents a novel scientific strategy for the systematic invention of new engineering materials with unprecedented structural and functional properties. *CME* will achieve this goal by intimately merging and advancing the research areas *Combinatorial Materials Research* and *Scale-Bridging Materials Modelling*.



The research within the proposed Cluster of Excellence is based on a continuous, iterative exchange between high-throughput simulation and high-throughput experimentation across all length scales and defines a new approach to the systematic invention of new engineering materials.

CME accounts for the evolution of our field, where materials science and engineering is entering a new era in which the traditional approach of observation and validation of materials performance will be replaced by predictive engineering of materials and functionality. *CME* represents a novel scientific strategy for the systematic invention of new engineering materials. *CME* will use the platform of the Materials Research Department (MRD) at the RUB, promotes interdisciplinary research and intends to improve substantially on traditional trial-and-error approaches. The performance of key materials which are needed for solving the grand challenges of mankind – energy, transportation, health and the environment – is central to *CME*. Integral to this approach, is speeding up discovery and progressing seamlessly to application and exploitation in the selected areas of research.

G. Eggeler. A. Ludwig, R. Drautz
■ *www.cme.rub.de*

SFB-TR 87 Pulsed High Power Plasmas for the Synthesis of Nanostructured Functional Layers

With structures of 30 nm and smaller, aspect ratios of 1:100 and more, modern plasma technology blazes the trail for many branches. Within the Sonderforschungsbereich-Transregio 87 (speaker: Prof. Dr. Peter Awakowicz) the Bochum plasma community is cooperating with materials science and engineering departments of RWTH-Aachen (co-speaker: Prof. Dr. K. Bobzin), the Institute for Materials at Ruhr-Universität Bochum and the chair for technical chemistry at University of Paderborn. Figure 1 shows the strong interdisciplinary cooperation within the SFB-TR 87. This cooperation concerns mechanical and electrical engineering, physics, chemistry and materials science. By investigating *new high power pulsed plasma sources for thin film deposition* with sophisticated *plasma diagnostics and simulation tools*, correlations to new materials properties will result. For the first time, basic materials science with ab-initio simulations and thin film engineering developed at new high power pulsed plasma sources is combined with basic plasma physics and engineering. In addition, these fundamental investigations are demonstrated for two examples, the deposition of *abrasion resistant coatings* on metal substrates and of *diffusion barrier coatings on polymer materials*.

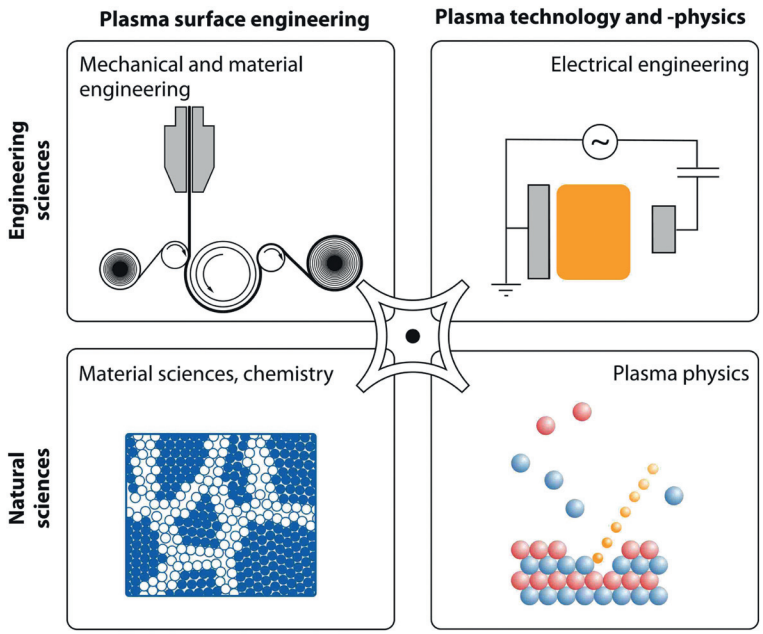


Figure 1: Interdisciplinary cooperation within the SFB-TR 87

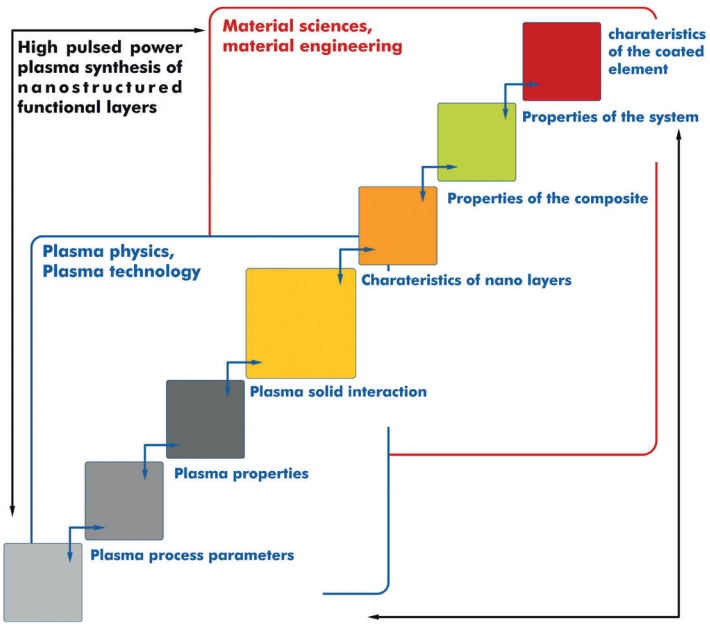


Figure 2: Cooperation within the SFB-TR 87 "From basic plasma properties to the coated mechanical part or component".

In Figure 2, the objectives and the cooperation scheme of the SFB-TR 87 are outlined. To start with the lower left corner, plasma process parameters are investigated which deliver the most relevant properties for the designed coating as ion energies on the substrate or species densities and species temperatures within the plasma bulk. On the third step, different groups of the SFB-TR 87 are investigating the plasma-solid interaction which is responsible for many characteristics and properties like the thin film growing dynamics or the adhesion on the substrate. In order to understand the properties of the deposited nano layers like for example their chemical composition, the surface energy or the plasticity or elasticity as a functional entity of both, the layer and the substrate, many different surface analysis methods are applied. At the fifth step in Figure 2, several groups in the SFB-TR 87 are investigating the characteristics of the systems which comprise the functional layers and the measuring system, like internal stress or the crystalline structure. System properties like abrasion resistance or corrosion resistance of coated metal substrates or diffusion barrier properties of coated polymers are in the focus at the sixth step. Last but not least a coated part or component like the heavily loaded extruder screw in a polymer processing tool will be analyzed and studied in the seventh step.

All these steps are treated in parallel. The main focus is placed on the interfacial definition and cooperation between the aforementioned steps. By doing so, different disciplines in science and engineering are working together in a very promising field of materials surface science with the vision of simulating, depositing and analyzing functional nanostructered thin layers with predictable properties.

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Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

Materials Modelling across the Length Scales

ICAMS is a research centre at the Ruhr-Universität Bochum. ICAMS focuses on the development and application of a new generation of simulation tools for multi-scale materials modelling with the aim of reducing development cost and time for new materials. Within the approach taken by ICAMS, the different length scales that are relevant for materials - from the atomic structure to macroscopic properties - are bridged by an interdisciplinary team of scientists from engineering, materials science, chemistry, physics and mathematics.

ICAMS is linked to the Institute for Materials (RUB), the Department of Ferrous Metallurgy (RWTH-Aachen) and the Max-Planck Institute for Iron Research (Düsseldorf). ICAMS is funded by ThyssenKrupp Steel Europe AG, Bayer MaterialScience AG, Salzgitter Mannesmann Forschung GmbH, Robert Bosch GmbH, Benteler Stahl/Rohr GmbH, Bayer Technology Services GmbH and the state of North-Rhine Westphalia as well as the European Union. Through bundling expertise on modelling and simulation of materials across all length and time scales at ICAMS and the advanced study groups with experimental support as well as input and insight from industry, ICAMS is in a unique position that will allow it to fast-track the development of advanced multi-scale modelling methods.

ICAMS is now in its third year and has published more than 180 contributions in scientific journals or books since 2008.

Current research highlights of the ICAMS departments are:

Simulation of the influence of hydrogen and other light elements in iron and steel

The aim of this project is to obtain a multiscale description of the interaction of hydrogen with metals and alloys. Properties of nanostructured materials are simulated by bridging methods ranging from the atomistic to the microscopic length scale. Aims are the identification of failure mechanisms and suggestions to prevent failure of iron and steel based materials.

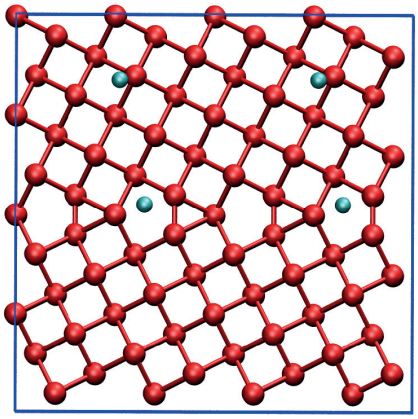

Figure 1: Atomistic simulation of the mobility of hydrogen in the presence of a grain boundary.

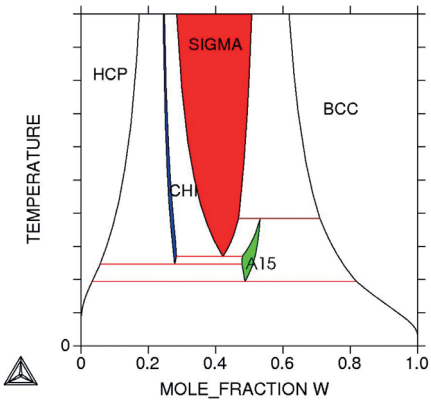

Figure 2: Prototypical Re-W phase diagram calculated from ab-initio input data.

Thermodynamic Database Development

The simulation of phase diagrams from first-principles calculations allows the description of thermodynamic properties of steels and alloys to be improved, especially for systems that are experimentally difficult to characterize. The data obtained in this way are used for the re-parameterization of thermodynamic databases (SAPIENS) and are the basis for the description of microstructural evolution, like the prediction of Laves phase growth.

Mechanical Properties of Grain Boundaries

Numerical models for the prediction of mechanical properties of interfaces in crystalline materials, like sliding or separation of grains or phase boundaries are developed. These models will allow the mechanical properties of nanostructured materials to be predicted and will provide fundamental understanding of the deformation and failure mechanisms of materials.

Nano Grain Growth

The successful simulation of grain-growth in nanostructured materials is a recent example for the description of crystalliza-

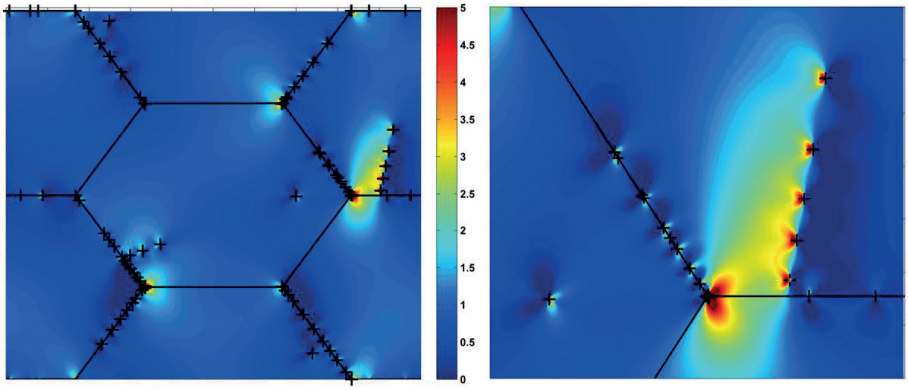

Figure 3: Color-coded tensile stresses (in GPa) in a polycrystalline aggregate. Plasticity is described on the basis of nucleation and motion of individual dislocations (marked as crosses). Grain boundary sliding caused by dislocation absorption is the origin of high stress concentrations at triple points, which in turn activate secondary dislocation sources.

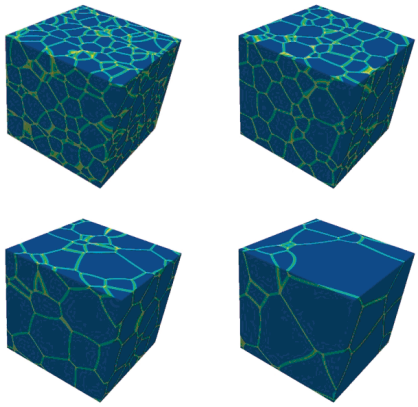

Figure 4: Mesoscopic grain growth simulations using the multi-phase-field model.

tion processes on the meso-scale. These processes are important for heat treatment and the prediction of mechanical properties of new materials.

ICAMS contributes to the following projects of the Materials Research Department:

- Mechanical testing of small scale specimens from functional and structural materials at elevated temperatures
- Doping of high purity diamond
- High temperature plasticity and microstructural stability in Ni-base superalloys: experiments and modelling
- Diffusion controlled reactions in and at single crystal Ni-based superalloys.

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CES Center for Electrochemical Sciences

As one winner of the HighTech.NRW competition the Center for Electrochemical Sciences (CES) of the Ruhr-Universität Bochum (RUB) was founded in October 2009 by the RUB and the Max Planck Institut für Eisenforschung Düsseldorf (MPIE), with additional financial support by ThyssenKrupp Steel. CES is regarded as a *Center of Excellence* with the task to ensure international competitive research in all aspects of *modern electrochemistry at the highest standard*. The key missions of the center are the coordination of large-scale research projects of its members, establishing cooperations with external partners from industry as well as other research institutions, and the promotion of young researchers by funding their research activities and offering training courses in electrochemistry on different levels.

"The central laboratory is open to all members and associated members."

To date CES has already completed its first successful year, which was mostly coined by building a strong foundation for future research. Therefore, a modern electrochemistry laboratory has been built up and equipped with various potentiostats including different electrochemical cells, electrochemical quartz micro balances, impedance spectroscopy, scanning electron microscopy, atomic force microscopy, surface plasmon resonance, Raman spectroscopy and dynamic light scattering. The central laboratory is open to all members and associated members. In addition, three junior research groups working on "Molecular Nanostructures", "Semiconductor Electrochemistry", and "Adsorption and Electrocatalysis" have been established by three young experts in their fields. Their research topics complement very well the work at the MPIE and RUB and therefore will enrich and broaden the existing expertise in electrochemistry.

Various research projects have already been initiated by the CES members. The projects are often connected to materials science like new materials for Lithium ion batteries or catalysts for the oxygen reduction reaction. CES is one of the partners of the project "Kompetenzverbund Nord: Steigerung der Kompetenz in Elektrochemie für die Elektromobilität". The project is dedicated to the understanding and improvement of materials used in Lithium-ion batteries. For the electrochemical characterization of materials such as functionalized carbon nanotubes or $LiFePO_4$, equipment of the central lab such as an atomic force microscope (AFM) and a scanning electrochemical microscope (SECM) have been transferred into a glove box to assure inert working conditions. The adaption of these techniques to inert conditions is also counted to the focus in instrument development within CES which include the development of space-resolved electrochemical methods or combining electrochemical methods with spectroscopy. Another focal point is seen in the area of theoretical electrochemistry with the aim to improve and adapt methods to electrochemical systems e.g. for the description of the oxygen reduction reaction or properties of semiconductors.

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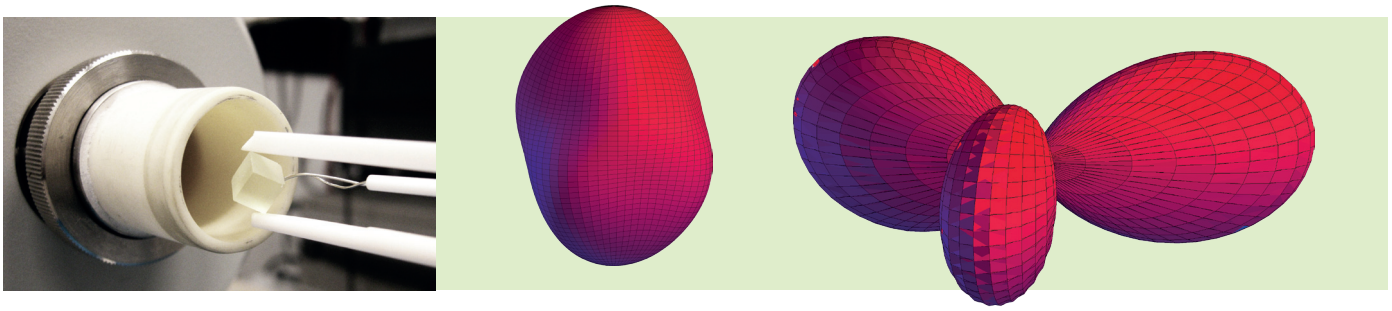

Fig. 1: Left: Sample mounted for high temperature resonance experiments. Middle and right: Spatial anisotropy of longitudinal elastic stiffness and piezoelectric effect, respectively, in a trigonal langasite single crystal.

Properties of Piezoelectric Materials for Harsh Environments

One focus of crystallographic research at the Institute of Geology, Mineralogy and Geophysics lies in the study of correlations between crystal structure and macroscopic electromechanical properties of piezoelectric single crystals with the long-term aim to develop new materials with optimized properties for technical applications. Electromechanical coupling effects in piezoelectric materials, i.e. the interactions between dielectric, piezoelectric and elastic properties as represented by up to 45 independent parameters at room temperature, allow for the conversion of electrical to mechanical energy and vice versa. Consequently, piezoelectric components made from single crystals or poled ceramics are used in many electronic devices today. Important applications are for example ultrasound generators / detectors and frequency filters in communication technologies as well as pressure and gas sensors in combustions engines and gas turbines. However, the use of piezoelectric crystals in harsh environments is still a major challenge because most materials at high temperatures suffer from phase transitions, electrical conductivity or anelastic relaxation effects.

In order to achieve self-consistent sets of electromechanical sample parameters as functions of frequency and temperature we developed an *acoustic resonance spectrometer* where these parameters are derived from resonance frequencies of a single freely vibrating sample with well-defined shape (Fig. 1). Currently, we are investigating the influence of chemical composition on the piezoelectric and elastic properties of natural tourmalines, the strong anelastic relaxation effects and structural instabilities in langasite ($La_3Ga_5SiO_{14}$) type crystal species and interactions of elastic waves with domain walls and short-lived ferroelectric nanodomains in relaxor ferroelectrics belonging to the $Ca_xBa_{1-x}Nb_2O_6$ family.

Another important topic of crystallographic research is the surfaces of solids which play a crucial role in corrosion, weathering, catalytic reactions and other processes where the solid-substrate interacts with gaseous, liquid or solid reactant. In crystals, the crystallinity of the surface of the substrate reflects the atomic order of the bulk, however, with termination effects leading to reorganization of the periodic order. In ambient environments the surface interacts with the atmosphere or liquids leading to layers of adsorbed molecules in registration with the crystalline substrate. Our focus of research is the structures of surfaces of bio-minerals such as calcite or apatite in their interaction with liquids and solutions containing molecules typical for living organisms, e.g. we have studied the surface structure of the (104)-surface of calcite covered with a molecular layer of the amino acid glycine. The same experiment was also performed with apatite as substrate. In this context we would like to analyse how organic molecules interact with the mineral surface and how minerals form at the interface. Similarly we studied the (001)-Zn-surface of ZnO and its interaction with water, an important catalytic support and coating material. At the ZnO-surface also, a water layer in crystalline registration with the metal-terminated (001)-face of the oxide support was found. The sorbate layer of the solvent water should play an important role in corrosive or catalytic reactions occurring at the crystal interface. The analysis of the surface structure is carried out with grazing incidence X-ray diffraction (GIXRD) using the scattered intensity in the truncation rod for structure analysis.

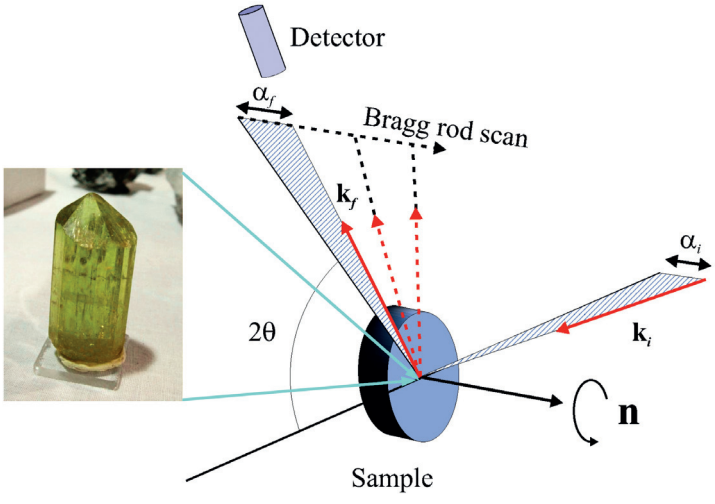

Fig. 2: Typical apatite crystal shown together with the experimental set up used for GIXRD experiments for surface structure analysis.

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

IMPRS-SurMat: Successful Evaluation and Extension for Further Six Years

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

Evaluation and extension

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

Scientific Scope

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

Outlook

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

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

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

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Short News

New Junior Professors at Ruhr-Universität Bochum

Junior Professor of Inorganic Nanomaterials for Photocatalysis, Photoactive Materials Group, Inorganic Chemistry II, Ruhr-Universität Bochum, Germany (since 01.07.2010)
- *Email: Radim.Beranek@rub.de*
- *Internet: www.rub.de/photochem*

The Beránek group's research interests combine aspects of synthetic chemistry with aspects of physico-chemical characterization and utilization of novel materials as building blocks for functional photochemical architectures and devices. Currently the focus is on the development of chemistry-based approaches to solar energy conversion, particularly the synthesis of novel nanostructured and hybrid materials for use in photochemical systems capable of harnessing solar energy to produce electricity (solar cells) or drive useful chemical transformations (for example, hydrogen production or the degradation of harmful pollutants).

Junior Professor of Microstructure of Materials, Chair of Materials Science and Engineering, Faculty of Mechanical Engineering, Ruhr-Universität Bochum, Germany (since 01.07.2010)
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Understanding of the relationship between materials microstructures and mechanical and functional properties, and the effect of chemical composition, processing parameters and microstructure, is a fundamental aspect of materials engineering. The current focus of my research is the investigation of these relationships in tempered martensite ferritic steels for high temperature applications such as power plants. In particular, I am investigating the effect of microstructure on high-temperature cracking using electron backscatter diffraction in the SEM, and developing techniques to characterise the microstructural degradation that takes place during long-term exposure to high temperatures.

In addition to my research activities, I am also involved in teaching in the new ICAMS Materials Science and Simulation Master Program.

Materials Research Department

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