Materialwissenschaften

Ruhr-Universität Bochum

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G. Eggeler, C. Bock

Intro

Materials Science and Engineering (MSE) is one of the research priorities at the Ruhr University Bochum (RUB). It is based on a joint approach from engineering and science departments to contribute to a better understanding of basic and applied problems related to the use of materials in advanced technologies including automotive and energy engineering, electronics, biomedical engineering and aeronautics. There is a special focus on the role of microstructure in governing the structural and functional properties of materials and on material properties which are dominated by the presence of internal and external interfaces. The thematic priority MSE combines efforts from different research fields like synthesis and processing, characterisation, and property assessment on all length scales ranging from atomistic (0.1 nm) to macroscopic (0.1 mm) distances. Moreover, modern materials science and engineering benefits from a strong interaction between experimental and theoretical approaches. The latter involve materials modelling on all length scales (atomistic, mesoscopic and macroscopic) with the objectives to determine material properties from first principle calculations and to predict the behaviour of complex material systems.

MSE as a research area has a long and strong tradition at Ruhr-University with materials scientists from different departments working together and sharing expensive research infrastructure. In 1997 all materials scientists at RUB, associated with the faculties of Mechanical Engineering, Electrical Engineering, Civil Engineering, Physics and Astronomy, Chemistry and Geosciences, joined forces and organised materials science research in the frame of the 'RUB Materials Forum'. The main objective of the Materials Forum is to promote interdisciplinary MSE research and teaching at RUB. Outstanding research track records were established in four areas: (1) engineering materials and mechanical properties, (2) nanostructures and nanomaterials, (3) thin films and (4) surface chemistry. State-of-theart research in these areas generally involves (i) advanced interface characterisation tech-

niques, (ii) the assessment of interface related properties, (iii) theoretical understanding and an experimental investigation of elementary processes at interfaces and (iv) interface engineering. It also requires modelling activities which reflect the state-of-the-art in theoretical chemistry/physics and in the development of computational/numerical methods.

The discussions within the *RUB Materials Forum* have initiated a number of successful research and teaching activities which we briefly describe in the present brochure (the 5^{th} of its kind since 1997). Please do not hesitate to contact us in case you need any further information or in case you wish to establish a link with RUB material scientists.

G. Eggeler

Sonderforschungsbereich 459: Shape Memory Technology

Shape memory alloys (SMAs) are potential candidate materials for many interesting applications. They show thermal and mechanical shape memory which are both related to the martensitic transformation which is a diffusionless solid state transformation. In a martensitic transformation, lattice shear processes are associated with cooperative movements of atoms. Although the displacement of each atom is not large, the martensitic transformation can result in a shape change, as all atoms within one domain or variant move in the same direction. As a result, shape memory alloys have unique properties including the oneway effect and pseudoelasticity. New shape memory

applications (couplings, sensors, actuators, deploying devices, implants, thin films, medical devices ...) can only succeed when two basic requirements are fulfilled. High quality materials with good reproducibility of structural and functional properties must be available at reasonable prices and design principles must be defined which make the best use of SMA properties without exceeding the physical limitations of the materials. Progress in the science and engineering of SMAs can therefore only be achieved through a simultaneous effort in the research areas (A) fundamentals of SMAs, (B) engineering design and applications of SMAs and (C) processing and manufacturing of SMAs. In the collaborative research center SFB459, scientists from engineering, physics, chemistry, crystallography and medicine join forces to achieve breakthroughs in shape memory technology. In the third three year funding period of SFB459, nineteen scientific projects collaborate closely to progress the field. To give an example, researchers of SFB459 apply transmission electron microscopy (TEM) to study the microstructural features associated with the martensitic transformation in Ni-rich NiTi single crystals. Four TEM micrographs from an in-situ cooling experiment are shown. In micrograph (a) the low temperature phase B19' (dark) forms in the interface between a Ni₄Ti₃ precipitate (bright) and the matrix (marked by white arrow). In micrograph (b) the B19'-phase grows along the precipitate/matrix-interface. Then, in a microscopic burst like event, the region left from the precipitate transforms into B19' (micrograph (c)). And subsequently, in micrograph (d), the region on the other side of the precipitate transforms into B19'.

For further information see www.rub.de/sfb459



Figure 1: Series of four TEM micrographs showing the fomation of B19' in Ni-rich NiTi single crystals on cooling from 193 to 185 K.

U. Kunze

NanoCentre: Background and Objectives

The science of nanostructures and nanomaterials represents the youngest branch of materials science. It offers a wide and multi-faceted field for basic research with interdisciplinary challenges for chemists, physicists, and engineers. Furthermore, the nanoscience field has a strong but unexploited potential for applications ranging from surface treatments at atomic resolution to the development of novel electronic devices and structures. Based on this background and on the long tradition in materials science the Ruhr-Universität at Bochum a new initiative on nanoscale materials started in 2002 named "Centre of Excellence Nanostructures and Nanomaterials", abbreviated "NanoCentre" (speaker: Prof. Dr. U. Kunze). 14 members and their groups from four departments -Chemistry (5), Physics (5), Electrical Engineering (2) and Mechanical Engineering (2) – successfully cooperate on natural nanoscale materials, self-organized nanostructures (bottom up) and lithographically defined structures (top down). The bottom-up strategy is

pursued by self-assembling molecules in forming layers and clusters, precursor chemistry, metal-organic precipitation, molecular-beam epitaxy, atomic-layer deposition, and plasma deposition processes. Nanoscale patterning by electron-beam lithography is the main technique of the top-down strategy, complemented by focussed ion beam and scanning probe techniques as well as self-adjusting methods. These preparation techniques are accompanied by analytical methods like electron microscopy, scanning probe microscopy, spectroscopy and scattering techniques.

The rich variety of nanoscale material systems like colloidal Au clusters, ordered pentacene layers, InAs quantum dots, InN nanowhiskers, C nanotubes, mesoporous silica, or Co/Cu superlattice nanowires, is investigated with respect to electronic, magnetic, optical, mechanical, or chemical properties for novel applications in, e.g., information technology, sensor techniques, or catalysis. Particular effort is spent on (opto-) electronic devices, which exploit their spin or wave properties of the electrons in addition to or instead of their charge.

Finally, it is essential to recognize possible applications of such materials at an early stage and to fathom their potential. Crucial issues resulting from stability and reliability of nanoscale functional devices, which suffer from many factors associated with their small size, are also subject of joint projects.

The NanoCentre represents an excellent environment for young scientists. Students

learn to communicate with researchers from other disciplines with the objective to share methods and infrastructure to reach their research objectives faster. Thus the NanoCentre members have arranged an interdisciplinary study program, containing lectures, laboratory courses, and workshops, which opens a specific access to the nanoscale research area.

For further information see www.nanocenter.rub.de



Figure 2: (a) Scanning electron micrograph of a cascaded ballistic rectifier prepared from a GaAs/AlGaAs heterostructure. Upon applying an input voltage $V_{ij} = V_i \cdot V_j$ ($V_j = -V_i$) between either single (ij = 12 or 34) or both (ij = 12+34) pairs of current injecting branches a rectified output voltage $V_{LU} = V_L \cdot V_U$ is found between the voltage probes L and U. (b) If V_{ij} is applied to both pairs of current injecting branches the voltage rectification efficiency $\eta = V_{LU} / |V_{ij}|$ is enhanced.

H. Zabel

Sonderforschungsbereich 491: Magnetic heterostructures: spin structures and spin transport

Heterostructures consist of combinations of different materials, which are in contact through at least one interface. Heterostructures combine different physical properties which do not exist in nature. Examples are semiconductors/ metals, superconductors/ferromagnets, or ferromagnets/antiferromagnets. These combinations promise to jointly display new physical properties different from any single one of them. Heterostructures are generated by stackwise deposition of different material layers via molecular beam epitaxy, via sputtering, or laser deposition, and by lateral structuring using electron-beam and ion-beam techniques. The SFB 491 (Speaker: Prof. Dr. Dr. h.c. Hartmut Zabel) investigates the basics of future information- and communication technologies based on the spin of electrons. Progress in this field requires to bridge literally semiconductor- and

(H. Zabel continued)

metal-physics by common interfaces in spintronic heterostructures. This is achieved by the growth of complex magnetic heterostructures; by lateral structuring on length scales down to a few nanometers; by investigation of new physical properties through proximity-effects acting between ferromagnetic layers and antiferromagnetic, ferroelectric, semiconducting or superconducting layers; and by optimization of spin-polarized electron transport in heterostructures or by spin-injection into semiconductor materials.

The SFB 491 has been funded by the DFG since January 2000 and is now in its third funding



period since January 2006. About 50 scientists are working within the SFB 491, 27 of them are young researchers (PhD students and postdocs) supported by research grants from the DFG.

The SFB is not only devoted to state-of-the-art research activities but also to the education and training of its PhD students through special lectures, summer schools, seminars and colloquia relevant to the goals of the SFB491. Furthermore a number of international workshops/symposia are organized each year on timely topics.

For further information see www.sfb491.de

Figure 3: Atomic force microscopy (left) and magnetic force microscopy (right) of an array of magnetic dipoles arranged on a square lattice. The array was prepared by electron beam lithography from a NiFe-permalloy film using a negative resist. The orientation of the magnetic dipoles may be used for information storage.

Ch. Wöll

Sonderforschungsbereich 558: Metal-substrate interactions in heterogeneous catalysis

Small metal particles supported on oxides exhibit very interesting electronic and chemical properties which deviate significantly from the corresponding bulk properties, in particular if the size of the metallic deposits reaches the nano-regime. It is the objective of the Sonderforschungsbereich (SFB) 558 to investigate the chemical activities of deposited metal clusters as a function of size and the interaction with the oxide substrate. The main motivation for this work comes from the pronounced importance of oxide supported metal particles for heterogeneous catalysis an important case is methanol synthesis.

In the framework of this Sonderforschungsbereich (Speaker: Prof. Dr. Christof Wöll) a number of groups from Technical Chemistry, Inorganic Chemistry, Physical Chemistry and Theoretical

Chemistry collaborate to study the importance of metalsubstrate interactions using a number of rather different approaches. Of particular importance is the precise experimental characterization using microscopic and spectroscopic methods as well as the theoretical description using both, precise ab-initio electronic structure calculations and molecular dynamics simulations.

Main topic of the third period of funding (July 1, 2006 to June 30, 2009) will be the characterization of metalsubstrate interactions in the case of small metal particles on oxide supports, in the foreground of this investigations will be the systems Cu/ ZnO and Au/TiO₂. The precious metal gold reaches a spectacular chemical activity in the case of nano-sized particles.

The co-operation of the SFB

558 with various industrial companies will be continued within the frame of the Transferbereich titled "CVD preparation of Cu/Zn/Al supported catalysts for methanol

synthesis", which is associated to the SFB 558.

For further information see www.sfb558.de





Figure 4: Single particles of a ZnO catalyst powder are addressed with the tip of a scanning tunneling microscope (STM) under the control of a scanning electron microscope (SEM). The STM image on the right shows atomic double steps on a mixed-terminated $ZnO(10\overline{10})$ surface of a single ZnO nanoparticle.

B. Stöckhert, C. Trepmann

Sonderforschungsbereich 526: Rheology of the Earth

SFB 526 "Rheology of the Earth" (present speaker: Prof. Dr. W. Friederich) is dedicated to the mechanical behaviour of Earth materials on all length and time scales, and at conditions from the Earth's surface to its deep interior, with a broad methodological spectrum. There is large scientific overlap with materials science and engineering research especially in the field of deformation and microfabric. Rocks are polyphase materials, mainly composed of silicates. They are deformed by tectonic processes, within seconds during earthquakes and very slowly during continuous motion of tectonic plates. High temperatures in

the Earth's interior cause annealing. Both deformation and annealing processes at given temperature, stress and pressure conditions leave a specific microstructural imprint in rocks, which can be compared to the results of laboratory experiments. These microstructures are the key to assess mechanisms and conditions at depths not accessible for direct analysis. Macroscopic geodynamic processes, such as plate tectonics, are correlated with micro- and nanoscale processes, as crystalline plasticity. Quantitative microfabric analysis of rocks relies on optical microscopy and electron microscopic technique, as in material

sciences. The figure shows the microstructure of a quartz crystal rapidly deformed at high stress in a laboratory experiment, which simulates loading by an earthquake at a confining pressure of 2 GPa and a temperature of 400°C, with subsequent annealing.

For further information see www.rub.de/sfb526



Figure 5: Orientation map showing the microstructure of an experimentally deformed and annealed quartz crystal.

A. Büttner

Max Planck Research School "Surmat"

The International Max Planck Research School for Surface and Interface Engineering in Advancd Materials (speakers: Prof. Dr. M. Stratmann, Prof. Dr. G. Eggeler; coordinator: Dr. A. Büttner) is a collaborative project involving the Max Planck Institute for Iron Research in Duesseldorf. the Max Planck Institute for Coal Research in Muelheim, and four departments of the Ruhr University in Bochum. Furthermore the State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, the Department of Materials, University of Science and Technology, Beijing, and the Department of Chemistry, Fudan University are involved in this Research School. Since the official start in April 2004 the IMPRS-SurMat acceptet 29 doctoral students and affiliated students

from 14 nations.

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. SurMat covers topics ranging from fundamental scientific issues to engineering applications, including material stability, local reactivities on heterogeneous surfaces, and the sophisticated tailoring of surfaces by thin film and nano-structuring techniques.

As the close collaboration between science and engineering departments is the key factor for knowledge-based surface and interface engineering each PhD student will be supervised by more than



Figure 6: Surmat students from 14 nations at the campus of the Ruhr-University Bochum.

one member of SurMat and typically by members of both the surface science and the materials engineering community.

In addition to research, the interdisciplinary education of students is of particular importance for SurMat. The aim is that each student will gain an insight in concepts and methods of interface analysis and engineering that can be applied in various fields of advanced materials development. Therefore SurMat includes intensive teaching in four summer and winter schools and research symposia. The schools focuses 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. For further information see www.imprs-surmat.mpg.de

G. Meschke

Sonderforschungsbereich 398: Activities within the joint research project "Life Time Oriented Design Concepts" related to materials science

Reliable predictions of the safety of engineering structures require an adequate description of damage and time-dependent deterioration processes in the construction materials during the whole life-time of the investigated structure. Within SFB398, a number of numerical models are developed for the description of damage processes in cementitious and metallic materials induced by quasistatic and cyclic loading and of long-term degradation processes induced in cementitious materials by the transport of moisture, heat and corrosive chemical substances and associated chemical reactions, respectively. Although designed as part of a computational framework for structural analyses, the developed models take into

a)

b)

damage

account damage-induced microstructural changes on the micro-, meso- and macro-scale. In several projects, experimental investigations are performed to support the model development. The following projects related to material science of construction materials are performed within SFB398:

• Experimental investigation of mechanical degradation of normal-strength, high-strength and air-entrained concrete resulting from cyclic loading (Institute for Building Materials, RUB).

• Modeling of the formation and propagation of micro-cracks and their adolescence into macro-shear bands in polycrystalline materials (Institute for Continuum Mechanics, RUB).

Chemical dissolution of cementations materials

Chemo-mechanical degradation of a concrete beam

Macro-level Micro-level

leaching dissolution transport

Three point bending test

calcium ions

transport

of calcium

ions

load chemical

dissolution reaction

mechanical

• Damage detection in metallic specimens subjected to High Cycle Fatigue by means of acoustic emission techniques (Institute for Continuum Mechanics, RUB).

• Modeling of Ultra Low Cycle Fatigue in metallic materials subjected to large, cyclic loading. This type of failure is associated with large plastic deformations, growth and coalescence of micropores (Institute for Structural Mechanics, RUB).

• Experimental investigation of the deterioration of concrete resulting from frost action and attack of ammonium salt (Institute for Building Physics and Materials Science at University Duisburg-Essen)

• Hygro-mechanical modeling of concrete subjected to chan-

Nano-level

2 🜣

ging environmental conditions taking moisture transport and interactions with loadinginduced cracks into account (Institute for Structural Mechanics, RUB).

• Modeling of chemo-mechanically coupled processes in cementitious materials. This includes modeling of chemical dissolution processes at various scales (Figure 7a) and the modeling of chemically expansive processes in concrete. Multi-field analyses allow the prediction of long term structural degradation of concrete structures subjected to combined external loading and chemical attack (Figure 7b) (Institute for Structural Mechanics, RUB).

• Modeling of crack propagation on the meso-scale of concrete in the context of multi-scale analyses. Figure 7c illustrates the crack propagation within a numerical model of the mesostructure of concrete (Institute for Applied Mechanics, RUB).

For further information see www.rub.de/sfb398

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Figure 7: On the modelling of chemo-mechanically processes in cementitous materials.