Dear Reader,

Welcome to the 10th issue of the MRD Newsletter, which reports on research projects of MRD members from different faculties of RUB. The MRD is closely cooperating with scientific institutions in the region, like the MPIE in Düsseldorf: the director of their new department “Structure and Nano-/Micromechanics of Materials”, Prof. Dr. Dehm, is simultaneously Professor at the “Institut für Werkstoffe”, Faculty of Mechanical Engineering of RUB.

This time the articles of the Newsletter share the focus on small scale materials (thin films, nanoparticles, qubits) and their mechanical, electrical and chemical properties. An additional article reports on understanding complex intermetallic phases by atomistic simulations. Furthermore I am happy to report that the “Institut für Werkstoffe” and “ICAMS” have moved to the new IC building and are thus now in closest vicinity on the campus (ICFO, ICFW).

Finally, the detailed planning for the new research building “ZGH” is advancing and the “Materials Days 2013” (4.–6.11.2013) will host the “International Workshop on Interface-dominated Materials”, which is part of the scientific preparation for “ZGH”.

Yours Sincerely,

A. L.  

Prof. Dr.-Ing. Alfred Ludwig

Editorial

Nano-/Micromechanics of Materials

The new department Structure and Nano-/Micromechanics of Materials at the Max-Planck-Institut für Eisenforschung GmbH (MPIE) aims to understand deformation mechanisms at small length scales in complex and miniaturized materials.

The mechanical challenges for structural materials applications at macroscopic length scales are apparent; while for materials employed in miniaturized systems – such as microelectronic devices or micro-electro-mechanical systems (MEMS) – the functional properties are of primary concern. However, the mechanical properties should not be overlooked as any mechanical damage may cause failure of functional devices. Frequently, the material components of functional devices/systems are exposed to extremely harsh mechanical conditions: Thin film structures for flexible electronics are cyclically bended and folded, metals and insulators in semiconductor devices are exposed to repeated thermo-mechanical loading by Joule heating or ambient temperature fluctuations, interfaces between materials of different bonding characteristics are supposed to remain intact, and miniaturized energy harvesting systems often endure aggressive chemo-mechanical environments preventing long-lasting and efficient service. To obtain quantitative mechanical data of small structures is a challenge due to the tiny material dimensions of a few micrometers or even less. However, quantitative mechanical tests are required to resolve the mechanical properties of miniaturized materials and to shed light on the deformation mechanisms which are usually altered compared to their bulk counterparts. Surfaces and interfaces impose constraining effects which need to be understood to predict the behavior of miniaturized materials and devices.

A cornerstone of the research work of the new department is the combination of quantitative and often self-build miniaturized mechanical tests with microstructure characterization techniques. This combination provides basic information on the underlying deformation mechanisms and will be illustrated in the following with a few current research examples.
Fig. 1 shows a scanning electron microcopy (SEM) image of a thin metallic film on a flexible polyimide substrate, which was strained inside the SEM until fracture of the film occurred. The in situ tensile testing experiment reveals cracks and buckles. Buckles form due to the geometrically necessary dislocations locally stored in the grains. The in situ low cycle fatigue experiment performed at 400 °C allows to control the stress triaxiality and to determine the mechanical properties of the material. Further, the particle size, shape, and density can be controlled by changing the type of liquid or laser parameters such as laser fluence, wavelength, pulse repetition rate, pulse width, etc. Fig. 1 shows a schematic of the laser ablation process in liquid media that has been used in our experiments.

During the process, a bulk target is placed in a glass vessel which is filled by a liquid. A short (< 0.1 μm) or ultra-short (< 10 fs) laser pulse is focused on the target. During loading and unloading, the nanoparticles absorb the laser light, (1064 nm wavelength, 50 μJ pulse energy and 1 kHz repetition rate). The laser ablation is instantaneous and the nanoparticles are formed homogeneously after the process. Moreover, no additional chemical precursor is necessary, the chemical composition of the nanoparticles corresponds to that of the ablated target material and resulting nanoparticles are chemically pure. Further, the particle size, shape, etc. can be controlled by changing the type of liquid or laser parameters such as laser fluence, wavelength, pulse repetition rate, pulse width, etc. This process allows to control the local deformation processes. Thus, detecting and understanding the underlying mechanisms locally may turn out to be a key to improve the mechanical performance and lifetime not only of miniaturized materials but also of macroscopic materials.

With this short overlook I would like to present a first impression on some of our activities in the field of micromechanics of materials. Further information can be found at our homepage (see: www.mpie.de). With my advisor professorship at the RUB and my membership in the Materials Research Department of the RUB I am looking forward to many fruitful collaborations.

Generation of Nanoparticles by Laser Ablation in Liquid

Nanoparticles are more than 100 times smaller than the diameter of a human hair and due to their properties are useful in a number of applications in plasmonics, chemical reactions and biomedical engineering. The main reason for these unique properties is the large surface-to-volume ratio, which increases with decreasing particle size. There are many possibilities to synthesize nanoparticles, e.g., wet chemical sol-gel process, gas phase hydrolysis, electrochemical etching. These methods show limitations for instance in the availability of precursor materials, the processability of complex materials, the dispersion of nanoparticles, agglomeration or ability to produce nanoparticles without impurities and toxic chemical precursors.

Laser ablation in liquids is an effective alternative method to generate pure nanoparticles with different size parameters (1–200 nm) in a variety of liquids. Compared to laser ablation in ambient air or gas atmosphere, the generated nanoparticles in liquid environment do not agglomerate and are dispersed homogeneously after the process. Moreover, no additional chemical precursor is necessary, the chemical composition of the nanoparticles corresponds to that of the ablated target material and resulting nanoparticles are chemically pure. Further, the particle size, shape, etc. can be controlled by changing the type of liquid or laser parameters such as laser fluence, wavelength, pulse repetition rate, pulse width, etc. This process allows to control the local deformation processes. Thus, detecting and understanding the underlying mechanisms locally may turn out to be a key to improve the mechanical performance and lifetime not only of miniaturized materials but also of macroscopic materials.

With this short overlook I would like to present a first impression on some of our activities in the field of micromechanics of materials. Further information can be found at our homepage (see: www.mpie.de). With my advisor professorship at the RUB and my membership in the Materials Research Department of the RUB I am looking forward to many fruitful collaborations.

An experimental setup for the investigation of the thermomechanical behavior of laser-based generation of nanoparticles has been designed at the chair of Applied Laser Technology (LAT). The setup is based on a fs laser source (Amplitude System, Tangerine, P = 20 W, λ = 1530 nm, f = 100 kHz). The laser is focused on the surface of metal target (NITI, 53.9.40.44 wt%), which has been chosen because of the high susceptibility of the material properties of the ratio of the two elements. The target was placed in a beaker filled with one of the following liquids: water, ethanol, acetone and ethyl acetate. The total ablation time in our experiments was limited by the concentration of nanoparticles in the solvent. If the concentration is relatively high, the nanoparticles may be absorbed by laser light, which is not advantageous while (i) the nanoparticles melt and agglomerate and (ii) laser energy reaches the target surface. In earlier experiments we have revealed an effective shielding of the particle growth due to an in-situ coating with organic molecules from the surrounding liquid.

Barckow and Oostendorf et al. generated NITI-NPs by a femtosecond laser system. They characterized the materials properties and the phase transformation of the NPs by differential scanning calorimetry (DSC) and demonstrated the phase transformation of the laser-generated NPs. In this case, the behavior of an ensemble of the laser-generated nanoparticles was studied. The aim was to deposit the NPs onto an implant surface and to determine their biocompatibility by incubation of human adhered-derived cells (ADMSCs) with NITI-NPs.

Recently, Transmission Electron Microscopy enables analysis of the crystalline structures of individual laser-produced nanoparticles. Fig. 2 shows TEM images of NITI-nanoparticles generated by laser ablation in water. The nanoparticles show spherical shape but in this case also a broad particle size distribution. By a special cooling holder (Gatan 660-DH), the nanoparticles were cooled and heated between −170 °C and 90 °C. At −94 °C a martensitic phase can be detected for a diameter of around 150 nm (specifically marked in Fig. 2 a). Upon further cooling to −125 °C the phase grows until final martensite structures are recognized (Fig. 2 b).
The Inorganic Materials Chemistry (IMC) research group at the Faculty of Chemistry and Biochemistry focuses on developing novel metalorganic precursors and utilizing them for the fabrication of thin films of functional metal oxides employing metalorganic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) processes. The nanostructured thin films are eventually characterized and evaluated for device applications.

The general motivation for exploring precursor chemistry for group IV oxides (TiO₂, ZrO₂, HfO₂) and rare earth (RE) oxides (Y₂O₃, Sc₂O₃, Gd₂O₃, Dy₂O₃, Er₂O₃) arises from the ever increasing interest in high-quality, uniform group IV or RE containing thin films as emerging materials mainly for applications in future generation microelectronic, optoelectronic or spintronic devices. While group IV metal oxides are relatively easy to synthesize and scale up, there are certain drawbacks associated with these compounds and therefore, over the last two decades as particularly suitable for industrial applications. Both techniques yield excellent coatings over large areas with complex surface geometries providing concomitantly a precise thickness and composition control. Apart from the some basic differences mainly related to film growth process, MOCVD and ALD have one in common and that is their strong dependence on the availability of suitable precursor chemistries. These two processes are governed by chemical reactions based on the precursor chemistry has continued through-out the years in pursuit of improved precursors to meet the demands of emerging applications for group IV oxides. In this context, the precursor development in terms of tuning group IV alkoxides and amide precursors with different chelating ligands such as ketoxetins, ketonamides, malonates, ureas, carbamates, guanidinates and amidinates offer more choice for CVD and ALD applications. It was demonstrated that tiny changes in the ligand periphery of metal complexes can significantly influence the precursor properties which in turn can have a distinct bearing on the film properties.

The mixed alkoxides of group IV were volatile, less sensitive to air and moisture and thermally stable compared to their respective parent alkylamides, possess suitable reactivity for ALD applications and yielded good quality group IV oxides under the adopted MOCVD/ALD process conditions and in some selected cases tested successfully in industrial scale reactors for the growth of group IV oxides (Fig. 1).

Compared to other functional metal oxides, there are very limited reports available on the MOCVD and ALD of RE oxide thin films and this can be attributed to the lack of suitable RE precursors with appropriate physico-chemical properties in terms of volatility, reactivity stability and decomposition characteristics. Therefore the focus of our work was to design and develop novel RE compound classes with improved precursor-chemical properties with respect to volatility, thermal stability and suitable chemical reactivity using appropriately tailored ligand systems. For example, the N,N-di-alkyl-guanidinates were selected as promising candidates. The resulting RE-tris-guanidinates turned out to be excellent precursors for MOCVD and ALD of RE₂O₃ thin films and can be treated as benchmark precursors for RE containing thin films (Fig. 2).

Having selected the most promising candidates among the new compound classes, their suitability as precursors for MOCVD and ALD of RE oxides (Sc₂O₃, Y₂O₃, Gd₂O₃, Dy₂O₃, Er₂O₃) was successfully explored. Of particular significance is the first ever demonstration of a water-assisted true ALD RE₂O₃ process developed using the novel tris-guanidinate RE precursors (Fig. 3). Employing a multi-technique approach, variations of the growth characteristics and film properties with deposition temperature were studied in terms of crystalinity, structure, surface roughness, composition, and electrical properties. Device quality RE₂O₃ thin films were obtained with high growth efficiency simply by using the RE guanidinate class of precursor in combination with water and thus avoiding ozone as oxidant. From the precursor engineering point of view, the idea is not only to synthesize one or more arbitrary members of a particular precursor class, rather rationally introduce small and distinct changes in the ligand sphere in a systematic manner. This is very important since such an approach would provide knowledge on the relationship between the molecular structure of the precursors, their thermal characteristics and the properties of the resulting films.
The investigation of TCP phases in Ni-base single-crystal superalloys for phases lead to a degradation of mechanical properties. In order to gain a microscopic understanding of the trends in structural stability, we compute the formation energy of TCP phases with density-functional theory (DFT), with the expectation that these modelling techniques and contributions from ΔV/V are required to stabilize them. A primary advantage of high-throughput DFT calculations with an adjustable number of electrons is the straightforward determination of electronic structures for different values of N and ΔV/V. In collaborations with density-functional theory (left) to a canonical semiconductor material for electrical control of a solid-state flying qubit. Fig. 2: By laterally structured, finger-shaped top gates, the 2DEG is depleted under bias-adjustable finger gate in between which makes them more amenable to interferences. Here, we report the transport of electrons having also been transferred in Mach-Zehnder interferometers of quantum microtechnology. That is why, solid-state processors have also been transferred in Mach-Zehnder interferometers of quantum microtechnology. That is why, solid-state quantum computers have hybridized symmetric basis functions, and with V = 0.5 V, we realize a novel two-path interferometer which does not suffer from paths encircling the central region of the device (V = 0.5 V). This is in contrast with the conventional AB interferometer under low-energy excitations, the pseudo spin is then defined as a hybrid function of the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realization of such an electron in the upper and lower path, which makes them more amenable to interference and ruling out static interfering states. For simplicity, the realiza...
Seigo Tarucha in Ref. 

put currents as a function of $V$.

This flying qubit can also be used

gate length; $v$ technology. In addition to the ability to trans-

port the quantum mechanical states:

tunnel coupling and the difference of the
tunnel coupling. A rotation about the $z$-axis

is also possible by simultaneously controlling

and 5 about the $x$- and $z$-axis on the Bloch

Corresponding to the rotational matrix

operators $R_x(\theta)$ and $R_z(\phi)$ depicted in Fig. 4

and $I$-axis on the Bloch sphere.

Arbitrary rotation of the state is also possible by simultaneously controlling

the tunnel coupling and the difference of the

transmission phase between the two paths.

These results therefore demonstrate ideal

two-path interference with no phase rigidity, and the qubit can be controlled even

without a magnetic field. The flying qubit presented here is promising for quantum information

technology. In addition to the ability to trans-

fer the quantum information over a long

distance, it has a much shorter operation
time compared with other qubits in sol-

id-state systems. The operation time $t_{\text{op}}(L$ gate length; $v$ Frenkel velocity) is in the order of $10$ ps.

This flying qubit can also be used in combination with a static qubit.

Using a high-mobility heterostructure with a mean free path exceeding $100$

μm, it is possible to be principle able to integrate $100$ qubits because each quantum operation,

including two-qubit operation, is performed within a $1$

μm scale.

The author is indebted to his coauthors

Michisuya Yamamoto, Shintaro Takada,

Christoph Baur, Kenta Watarai, and

Seigo Tarucha in Ref. 24 who made the whole story possible and thus configured

with him wide parts of this article.

Meeting of the DGM Regional-

forum Rhein-Ruhr on 5.6.

September 2013 in Bochum

The DGM (Deutsche Gesellschaft für Mate-

rialwissenschaften) is a German national scientific society for researchers and developers from industry and academia in the area of materi-

als science and technology. Recently, DGM members have started to create local DGM centers, referred to as “DGM Regionalforen”. During the annual DGM day 2013, which was held in May at the Ruhr-Universität Bochum, a new DGM Regionalforum Rhein-

Ruhr was founded with Gunther Eggeler as its first speaker. All universities and research institutes from the wider Ruhr area with a research focus on materials science and engineering participate in the activity. Members come from RWTH Aachen, Ruhr-Universität Bochum, Universität Duis-

burg Essen, MPI für Eisenforschung, Uni-

versität Paderborn, DLR Köln, Universität Siegen, TU Dortmund and FZ Jülich.

The photograph shows members of the Regionalforum Rhein-Ruhr at their first meeting which was held on 5th September at the Horst Göse Saal in the Technology Center close to the Ruhr-Universität Bochum. One objective of the meeting was to discuss microstructure based materials design. Another objective was to present the activities of all regional of the materials education and research. At their first meeting the partners agreed on how to run the Regionalforum Rhein-Ruhr. Especially it was agreed to invite other partners to participate in events like lecture series and symposia. The dates and locations for the next two annual meetings were agreed upon (4th September 2014, FZ Jülich – Materials and energy, 14th September 2015, Universität Siegen – Materials for light weight structures). Most importantly, the DGM Regionalforum Rhein-Ruhr aims at providing a platform for discussing ideas, developing new research strategies and to strengthen the solidarity between material researchers in a competitive environment.

The MRD of the Ruhr-Universität Bochum fully supports the activities of the DGM Regionalforum Rhein-Ruhr.

EU funds RAPID – Marie-Curie Initial Training Network at Ruhr University Bochum

The European Union has granted about 3.9 Mio. Euros for RAPID’s Marie-Curie Initial Training Network for a funding period of 4 years starting October 2014.

RAPID (Rheinische Atmosphärische Plasma Processing – Education network) is an interdisciplinary initial training network (ITN) at the intersection of chemistry, physics and microelectronics. The ITN aims particularly at the development of non-equilibrium reactive processes in atmospheric pressure plasmas. Thereby, the great success of low-pressure plasmas enabling a multitude of applications ranging from material synthesis, automotive and microelectronics can be repeated. This research and training is coordinated by the Ruhr University Bochum (RUB), Germany, and will be accomplished in a consortium involving 10 academic and 10 industrial partners from 8 European countries. For more details see www.rapid-rue.de

---

Imprint

Publisher: Materials Research Department Ruhr-Universität Bochum

Contact: Ruhr-Universität Bochum Materials Research Department Prof. Dr.-Ing. Alfred Ludwig Universitätstrasse 150 D-44801 Bochum Building ICFO, Floor 03, Room 225

Tel: +49 (0) 234 - 32-7492 Fax: +49 (0) 234 - 32-4490 E-Mail: mrd@rub.de Web: www.rub.de/mrd

Design: jungpartner.de