MM 23: Poster session

Time: Tuesday 14:45-18:00
Location: Poster B

**MM 23.1  Tue 14:45 Poster B**

**Nanotomography of Biomaterials** — *Stephanie Röper*, Christian Zeitz*, Christian Dietz, Nadine Drechsel, Andreas Bierwirth, Robert Magerle

1Chemische Physik, TU Chemnitz, D-09107 Chemnitz — 2Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken — 3Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Biomaterials such as bone and teeth are nanocomposites of proteins and minerals. At the molecular level, scale these materials have a stiff inorganic component (hydroxyapatite) that reinforces the soft organic matrix (type I collagen) through a recurring structural motif. To gather information of the nanometer scaled structure of these materials we use nanotomography. For this scanning probe microscopy (SPM) based method the specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode SPM after each etching step. In our experiments we focus on cortical human bone (embedded and native) and human teeth. The stepwise etching is done with a piezo-driven SPM with an automated setup. We will present our latest volume images of human bone and teeth and discuss new concepts for adjusting the imaging parameters to maintain a good imaging quality.

**MM 23.2  Tue 14:45 Poster B**

**Neutron Reflectometry Studies on Self-diffusion in Nano-Crystalline Fe Films: First Results** — *Sujoy Chakravarty*, Michael Horisberger, Thomas Gutberlet, Jochen Stahn, and Harald Schmidt

1Institut für Metallurgy, AG Materialphysik, TU Clausthal, Germany — 2Laboratorium für Neutronenstreuung, ETH Zürich & PSI, Villigen, Switzerland

Nano-crystalline metals show in comparison to their coarse grained counterparts improved mechanical properties like high hardness and fracture toughness and also interesting magnetic properties. At low temperatures mechanical deformation (grain boundary creep, grain boundary sliding), grain growth, and also thermal stability are essentially controlled or influenced by self-diffusion. For an understanding of these processes close to room temperature, we carried out self-diffusion measurements on nano-crystalline Fe films using neutron reflectometry. This method enables to determine extremely low diffusivities down to \(10^{-25} m^2/s\) and also extremely small diffusion lengths \(< 0.7 nm\). The temperature and annealing time dependence of the diffusivities is analyzed and explained in the framework of structural relaxation processes.

**MM 23.3  Tue 14:45 Poster B**

**Nitrogen Diffusion in Amorphous Silicon (Carbo)Nitride Probed by Neutron Reflectometry** — *Ewinn Hüger*, Thomas Gutberlet, Jochen Stahn, Michael Bums, and Harald Schmidt

1Institut für Metallurgy, AG Materialphysik, TU Clausthal, Germany — 2Laboratorium für Neutronenstreuung, ETH Zürich & PSI, Villigen, Switzerland

Amorphous bistable layers result from the influence of low energy light ions on silicon surfaces. The intermediate state can be protonated with hydrogen ions, forming an amorphous SiCNx layer. After protonation the layer can be annealed to either an all-carbonized layer or a SiCNx layer. With neutrons, a layer can be formed with a high nitrogen concentration. For neutron reflectometry, the layer is protonated and the nitrogen diffusion can be observed. To get high nitrogen concentrations, the layer is protonated and an amorphous SiCNx layer is formed. The neutron reflectometry setup is used to measure the nitrogen diffusion. The diffusion length of the nitrogen is measured and the results are in agreement with the theoretical predictions.

**MM 23.4  Tue 14:45 Poster B**

**Exciton formation in graphene bilayer** — *Raoul Dillenschneider*, University of Augsburg, Germany

Graphene, layers of two-dimensional honeycomb-array of carbon atoms, has attracted much interest these last few years due to its recent experimental accessibility and a wide variety of interesting properties. As the engineering application of the graphene layers attracts increasing significance, we need to explore, experimentally and theoretically, ways to enrich graphene's electrical properties and to control them. One way to achieve some control over the electrical properties is to change the number of layers and/or the bias applied across the layers. The bias can also potentially control the formation of excitons. Since the applied bias leads to the charge imbalance in the two layers, it is natural to suspect that the Coulomb attraction of the excess electrons and holes on opposite layers would lead to an exciton instability.

We consider the possibility of an excitonic instability for biased graphene bilayer in the framework of Hartree-Fock theory.

**MM 23.5  Tue 14:45 Poster B**

**Soft absorption edges studied with hard x rays** — *Henning Strenemann*, Christian Strenemann, John S. Tse, Juha A. Soininen, Yong Q. Cai, Serge Desgreniers, Timothy T. Pister, Noszohu Hiraoka, Achim Höhl, Andreas Schacht, Gerald T. Seidlen, Georgy Vankó, Simo Huotari, Kielo Hämäläinen, and Miett Tolan


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We consider the possibility of an excitonic instability for biased graphene bilayer in the framework of Hartree-Fock theory.

**MM 23.6  Tue 14:45 Poster B**

**Stability, electronic and magnetic properties of iron oxyhydroxides under high pressure: Insights from first principles** — *Katrin Otte*, Rossitza Pentcheva, and Jim Rustad

1Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — 2Department of Geology, UC Davis

Iron oxyhydroxides (FeOOH) play an important role in nature and technology, e.g. in binding heavy metals. The high pressure behavior of water containing minerals is important for understanding the processes in the Earth’s crust and lower mantle. Using density functional theory (DFT), we investigate the structural, electronic and magnetic properties of the iron oxyhydroxides-polyoxometalate (α-, β-, γ- and hp-FeOOH) under high pressures. We find that under ambient conditions goethite (α) is the lowest energy phase, while at high pressures the hp-phase becomes more favorable. The relative stability of the different phases follows the trend obtained from recent calorimetric measurements [1]. Bond lengths are in a good agreement with available experimental data. While in the ground state Fe\(^{3+}\)-ions are coupled antiferromagnetically, at high pressures a transition to a ferromagnetic alignment takes place in hp-FeOOH. At ambient conditions all AFM phases are insulating within the generalized gradient approximation.

The non-linearity of the electrical conductivity in the amorphous phase not only states to be the oldest of all puzzles in the field of phase change materials starting with Ovshinsky's discoveries in the 1960s, but also remains likely to be the most controversial one to this date. The most prominent effect in this context is the so-called threshold switching in the amorphous phase describing a sudden break down of resistivity in the presence of a critical electric field. Besides its scientific importance this effect is crucial for the currently most promising application of phase change alloys, i.e. electric memory (PCRAM).

Several theories about electronic transport of this class of materials have been proposed in the last decades, but there is still a lack of quantitative experimental data to prove them. To fill this gap in this work the mobility of the charge carriers is studied for several representative phase change materials. The dependence of the mobility on temperature and on the electric field is investigated and compared with existing theories. From this comparison insight into the mechanism of charge carrier transport is obtained.

High Kinetic Energy Photoelectron Spectroscopy Study of the Ni 1s Core Level and Satellite Structure — [1] Mihaela Gorgoi1, Svante Svensson2, Olof Karin3, Jan Runz2, Peter Oppeneer1, Franz Schafers1, Walter Braun1, Niels Martsensson2, and Wolfgang Ehrenhart1 — 1BESSY GmbH, Berlin, Germany, 2Uppsala University, Uppsala, Sweden

The Ni 2p level and its satellite structure have been studied since many years and the mechanisms behind this structure have been addressed in a large number of reports [1, 2 and references within]. In contrast, there is not a modern photoelectron spectrum of Ni 1s and the corresponding satellite structure. Using the HIKE facility at beam-line KMC1 at BESSY we have studied this core level using excitation energies from 9 keV to 12 keV. Our findings show that the satellite main line energy distance decreases for the Ni 1s level in comparison to the Ni 2p case. Our finding has important implications for the existing theoretical explanations of the classical Ni 1s core level problem and requires a revision of current models.

Critical Packing Fraction in Multicomponent, Glass Forming Metallic Liquids — Suresh M. Chatzithomas, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

Glass forming Ni59.5Nb40.5 and Ni60Nb34.8Sn5.2 have been investigated in their equilibrium liquid by quasistatic neutron scattering. These liquids exhibit extraordinary high packing fraction[1]. Structural relaxation shows stretching in time and extent of stretching depends on the temperature of the liquid. The self-diffusivity decreases about two orders of magnitude within 360 K. From the beta-relaxation, tau-scaling analysis of self-diffusion and mean relaxation times of the alpha-process the critical packing fraction of these liquids have been derived. Our results provide, for the first time, an experimentally observed value for the critical packing fraction in the glass forming metallic liquids and is in good agreement with mode-coupling theory prediction[2].

We gratefully acknowledge the financial support from SFB 602 TP B8 and DLR under grant No. 50WM0541.


Temperature dependence of elastic constants for the metallic glass Pd40Ni40P20 — Thomas Köpppe, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut Universität Göttingen, Germany

We have measured the elastic constants of bulk amorphous Pd40Ni40P20 in the temperature range from 2 K to 300 K. The measuring technique was the ultrasonic pulse echo method with a frequency of 6 MHz. With decreasing temperature a linear increase of the elastic constants is found. At lower temperatures an increasing deviation from the straight line is observed. The Poisson ratio shows a linear decrease with increasing temperature and deviation from that behavior at low temperatures also. This behavior is qualitatively the same as for single crystals and follows a 7 - law down to our lowest temperature. The measured loss is very small at low temperatures and depends mainly on the bonding agent. So bulk amorphous metals are transparent for ultra sound at low temperatures. This work was supported financially by DFG, SFB 602 and Leibniz Programm.

Influence of a miscut of Y2O3-stabilized ZrO2 single crystals on the formation of La2Zr2O7 islands by a vapour-solid reaction — Markus Andreas Schubert, Stephan Senz, and Dietrich Besse — Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The La2Zr2O7-forming solid state reaction between ZrO2 and La2O3 is of significance in view of solid oxide fuel cells degrading during operation by a reaction of this type, if ZrO2 is the solid electrolyte and if a La2O3-containing ternary oxide cathode is used. In model experiments, La2O3 vapour at 1200 °C directly reacts with an yttria-stabilized ZrO2 single crystal (YSZ) forming La2Zr2O7 (LZO) pyrochlore islands. Islands on YSZ(001) are square shaped and consist of four or eight slightly tilted domains. On YSZ(110), islands have a long edge along [110] and a short edge along [001] and four tilted domains. The tilt of the islands is a consequence of the misfit accommodation mechanism for a vapour-solid reaction with a large positive misfit of 5 %.

New experiments were performed to investigate the influence of the miscut angle on the favoured formation of special domains. YSZ(001) and YSZ(110) single crystals with a miscut angle of 4° were used. For YSZ(001) substrates the surface was rotated around a [100] or [110] direction, respectively, and for YSZ(110) it was rotated around the [110] or [001] direction. The relative orientation and morphology of the LZO islands were investigated in their equilibrium liquid by quasielastic neutron scattering. Glass forming Ni59.5Nb40.5 and Ni60Nb34.8Sn5.2 have been investigated in their equilibrium liquid by quasistatic neutron scattering.

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Eckert
Sakaliyska —
ics. This class of materials for instance possesses good electrical and thermal conductivities as well as considerable damage tolerance and temperature oxidation resistance.

The method of perturbed angular correlation (PAC) with implanted \(^{111}\)Indium as probe nuclei is successful in measuring the electric field gradient (EFG) of the A-site by using Indium containing MAX phases like Ti\(_3\)In\(_5\)C and Zr\(_2\)In\(_5\)C. These key- compounds provide a kind of fingerprint EFG that can be compared to other MAX phases which have no Indium in their structure. Special attention is payed to investigations of annealing parameters, thermal characteristics and behaviour under isostatic stresses.

MM 23.14 Tue 14:45 Poster B

Mechanical alloying and milling of Al-Mg alloys — •Mir\a raklis, K. Kumar Babu Suresh, S. Scudino, and Jürgen Eckert — IFW Dresden, Institut für Komplexe Materialien, Postfach 200116, D-01171 Dresden, Germany

Solid solubility extension far beyond the room temperature equilibrium value was achieved by mechanical alloying of elemental powder mixtures for the binary Al-Mg system in the range of 10 - 50 at.\% Mg. The Al(Mg) solid solutions are metastable and transform into the equilibrium phases during heating. No indication for the formation of the equilibrium phases (beta-Al\(_3\)Mg\(_2\) and gamma-Al\(_{12}\)Mg\(_{17}\)) during milling was detected. Similar results can be achieved by mechani- cal milling of intermetallic compounds. For example, for Al\(_60\)Mg\(_40\) mechanical alloying and milling yield the same metastable supersaturated solid solution as end product. Upon heating, the milled powders prepared from different starting materials display a complex behavior characterized by several exothermic events. At low temperatures, an increasing amount of Mg is rejected from the solid solution with in- creasing temperature. At higher temperature, a hexagonal phase with composition Al\(_3\)Mg\(_2\) is formed. The subsequent exothermic events correspond to formation and growth of the equilibrium beta-Al\(_3\)Mg\(_2\) phase. Finally, selected examples for the mechanical deformation be- havior of consolidated samples are presented, revealing encouraging properties regarding the combination of high strength and good duc- tility at room temperature.

MM 23.15 Tue 14:45 Poster B

New DFT-Investigations of Vanadium Silicides — Mike Thiem and •Shylo Geim — Forschungszentrum Dresden-Rossendorf, POB 51 01 19, 01314 Dresden, Germany

Vanadium and silicon form several binary compounds; the most well characterized structures have the compositions V:Si= 3:1, 6:5, 5:3, 1:2. Density-functional-calculations with a plane-wave basis for the valence electrons and norm-conserving pseudopotentials for the core-valence interaction have been carried out to investigate the structural properties and the phase stability for the experimentally known binary crystals. As the early transition metal silicides belong to the class of refractory materials, also the elastic properties were de- termined. It is furthermore shown that the electronic properties of the compounds depend on the composition.

MM 23.16 Tue 14:45 Poster B

The behaviour of different equations of state under pres- sure on the example of Claude Loose, Jens Kontus, Marcus Schwarze, Edwin Krokh, and Gerhard Heide — 1TU-Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany — 2TU-Bergakademie Freiberg, Institute for Mineralogy Breunhagensasse 14 09596 Freiberg, Germany — 3TU-Bergakademie Freiberg, Institute for Anorganic Chemistry, Leipziger Straße 29, Ger- many

We studied the effect of different Pseudopotentials and Equations of state (EOS) on the calculation of elastic properties (Bulkmodulus K and pressure derivative of the bulkmodulus K' ) and V\(_p\) at different pressure ranges. We also calculated transition pressures for the system AlN (wurtzite - rocksalt) and SiO\(_2\) (low quartz - coesite - stishovite) with respect to Pseudopotential and EOS. At low pressure all EOS gave similar elastic properties whereas increasing pressure leads to a divergence of about 10% while still fitting the same data. The transition pressure on the other hand depends only on the choice of Pseudopo- tential (LDA/GGA)

MM 23.17 Tue 14:45 Poster B

Hybrid electrode of carbon aerogels and metal oxides for electrochemical capacitors — •Volker Lohrmann, Henning Lörhrmann, Ingo Riedel, Gudrun Reichenauer, Matthias Wüchner, Carsten Diehl, and Vladimir Dyakonov — 1Bayesian Center of Applied Energy Research (ZAE Bayern), Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg, Germany — 2Lehrstuhl für Experimentelle Physik VI, Julius-Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg

Electrochemical capacitors (EC) fill the gap between conventional ca- pacitors with high power but low energy density and batteries with high specific energy density but rather low power density. There are two types of EC: Double-layer supercapacitors, which store charges electrochemically in the electrochemical double-layer between electrolyte and high surface area electrodes of activated hard carbon. In pseudo- capacitance supercapacitors the charge storage is of faradic-nature, e.g. redox processes in metal oxides. We have blended the organic precursor of a synthetic activated hard carbon (carbon aerogel) with metal oxide particles to be used as electrode for EC. The aim is to combine high pseudocapacitance and high faradaic capacitance with respect to Pseudopotential and EOS. At low pressure all EOS gave the same metastable supersat- uration point (LDA/GGA)

MM 23.18 Tue 14:45 Poster B

The Imaging Beamline at PETRA III — •Astrid Habiel, Felix Beckmann, Julia Herzen, Thomas Dose, Sven Utcke, and Andreas Schreyer — GKSS Research Centre Geesthacht

Since 2007 the GKSS is responsible for construction and operation of the Imaging Beamline at the new synchrotron source PETRA III at DESY. Due to the high brilliance (most brilliant X-ray source world- wide), the low emittance of 1nm rad (unrivaled for current storage rings at comparable high particle energies) and the high fraction of co- herent photons also in the hard X-ray range an extremely intense and sharply focused X-ray light will be provided. This advantages of the beam fulfill excellently the qualifications for absorption, phase contrast or holo tomography, for nano tomography and for high speed or in situ tomography. The first user operation of the facility is planned in 2009.

The Imaging Beamline will be structured into two experimental sta- tions for micro and for nano tomography. The X-ray energy will be tun- able between 5 and 50 keV. In the micro tomography hutch the inves- tigation of samples of some millimeters diameter in (sub)-micrometer resolution is planned. Here, fields of application encompass questions from materials science (e.g. analysis of pores, cracks, precipitations, phase transitions) as well as problems in the area of biology or medicine (e.g. structures of bones, tissues, teeth, plants).

The possibility to focus the X-ray beam into the nanometer range will be used for nano tomographic imaging. Therefore, a second hutch for two nano tomography setups is planned. For this setups spatial resolutions down below 100 nm are expected for micrometer sized samples.

MM 23.19 Tue 14:45 Poster B

Synchrotron radiation based microtomography (SRµCT) and neutron tomography (NCT) for materials science — •Felix Beckmann, Julia Herzen, Tilman Donath, Astrid Habiel, Thomas Dose, Jürgen Vollbrant, Heinz-Werner Schmitz, Phillip Klaus Praznas, and Andreas Schreyer — GKSS Research Centre Geesthacht, Germany

The GKSS Research Centre Geesthacht, Germany, is operating the user experiment for microtomography using synchrotron radiation at the Imaging Beamline PETRA III. A second hutch for neutron tomography in the Imaging Beamline at PETRA III is under construction. The beamline W2 was rebuilt. The outstanding feature of this synchrotron radiation beamline HARWI II is the use of high energy X-rays from 20 to 250 keV for materials science experiments. The features for micro- tomography at HARWI II and new enhancements and applications using lower photon energies at the wiglener beamline BW2 will be presented. The principle of the new neutron tomography facility GENRA 3 was extended by a setup for neutron tomography. Results performing SRµCT at HARWI 2 and NCT at GENRA 3 will be presented. The combination of neutron and synchrotron radiation
techniques will give new insight into the three-dimensional behavior of samples in materials science.

MM 23.20 Tue 14:45 Poster B
Forensic Science - Applications in Metal- and Material Physics — H. Katterwe — Kriminaltechnisches Institut / BKA, 65173 Wiesbaden
Forensic science refers to the examination of scenes of crime, recovery of evidence, laboratory examinations, interpreting of findings and presentation of the conclusions reached for intelligence purposes or for use in court. The paper describes forensic scientific cases, which can be solved by methods of applied metal- and material physics. Items and substances as bullets, cartridges, tool marks, fractures of metals and polymers, manufacturers marks and serial number restoration. Experiments which are employed include marks analysis, mechanical testing and recovering of erased characters by using aspects of solid-state physics, chemistry and engineering. Marking processes (die stamping, engraving, laser beam) change the microstructure of the metal (grains, slip bands, dislocations) or in cases of polymers the macromolecules around the marking become oriented (decreasing of the entropy). Methods used to restore erased numbers - both destructive and non-destructive - are described. ©newline Reference: Voss-de Haan. Katterwe, Simonos "Physik in der Kriminaltechnik", Physik Journal 2 (2003) Nr.9, 35-41.

MM 23.21 Tue 14:45 Poster B
The SKF Windows Expert Simulation Software SimCarb 2006 for Carburizing Case Hardening of Steels: a High-Performance CAE Tool for Industrial Process Optimization — Andreas Schreyer — SKF GmbH Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany
Although case hardening of steels has been technically applied for more than one century, regular variance comparison tests of state-of-the-art operations based on two-step boost-diffuse gas carburizing treatments for determining the accuracy level of process control show that the target parameters are not met reliably. Whereas, for instance, the carburization depth should lie within 0.1 mm around its desired value, in practice a three times higher discrepancy represents a good heat treatment result. Inadequate computer control of the process is caused by its high complexity. Critical quantities are, e.g., the composition-dependent diffusivity and the concentration-activity relationship of carbon in the specific steel. The prerequisite for successful process optimization is a powerful simulation tool. Fundamentals, menu-driven handling, and application of the SimCarb software are presented. Pick’s law of diffusion is solved by an implicit FD scheme under real boundary conditions. Material properties are selectable from large reference lists or freely defined by the user. In- and output are visualized online on the screen. Simulations can be saved in a special format. ASCII data export is supported. By advanced analysis, strategy development, feasibility studies and simulation runs, prediction and optimization of the heat treatment process are available. The software allows for detailed quality, sustainability and profitability improvement of case hardening.

MM 23.22 Tue 14:45 Poster B
Residual stress analysis of aluminium welds with high energy synchrotron radiation at the HARWI II beamline — René V. Martins
and Andreas Schreyer — GKSS research centre, Max-Planck-Str. 1, 21502 Geesthacht
In civil aircraft production advanced welding techniques, like laser welding or friction stir welding, are used to reduce weight and production costs. By the welding process residual stresses are introduced in the weld zone and the surrounding area. These stresses may depend on diverse factors and can have disadvantageous effects on the service performance of the weld. The use of high energy synchrotron radiation at the HARWI II beamline at HASYLAB, Germany, allows for a non-destructive and non-invasive residual stress measurement. The high energy X-rays allow for a high angular resolution for the peak position determination. The heavy load diffractometer allows making use of massive sample environments. For example laser beam welded t- and butt-joints were investigated with high spatial resolution. The large grain size of the specimen makes the measurements with high spatial resolution more difficult due to the poor grain statistics. The influence of the gauge volume size and grain statistics on the strain measurements were systematically investigated. For t-joint configuration two dimensional stress maps were calculated from the data. For the near future an in-situ FSW experiment is planned to investigate the metallophysical processes during the welding.

MM 23.23 Tue 14:45 Poster B
Field-driven evolution of stripe domains in magnetic shape memory alloy films — Nikolay S. Kiselev, Igor E. Dragunov, Aristide T. Onisian, Ulrich K. Rössler and Alexei N. Bogdanov
A phenomenological approach is used to describe the redistribution of martensitic variants driven by an external magnetic field in ferromagnetic shape memory materials. Real samples of magnetic shape memory alloys as the Ni-Mn-Ga Heusler alloys contain complex systems of crystallographic and magnetic domains [1, 2]. Magnetic reversal in such system is characterized by particular effects including the existence of 180-degree magnetic domain structures within the twin variants and the rotation of magnetic moments within magnetic domains in case of relatively weak magnetic anisotropies [1]. An elementary model for these complicated systems is proposed by using the "one-to-one correspondence" between magnetic domains and martensite variants [3]. For this model, we calculate stability ranges and evolution of equilibrium and metastable stripe states [3] and isolated twin-variants in thin single-crystalline plates. We discuss the applicability of this model to describe nucleation and magnetization processes in real samples.

MM 23.24 Tue 14:45 Poster B
Dependency of magnetic domain structures on stress and field history in bulk NiMnGa — Ryan Yu, Wai Lai, Jeffrey McCord, Rolf Schaefer and Ludwig Schultz — Leibniz-Institute for Solid State and Materials Research, P.O.Box 270116, Dresden D-01171, Germany
A study of the magnetic domain structure in bulk NiMnGa magnetic shape memory single crystals is presented. Polarization microscopy, using a magneto-optical indicator film technique, is employed to obtain the static magnetic domain patterns at all surfaces of bulk crystals. Different complexity of domain patterns is revealed with different twinning states (e.g. single variant state, two-variant state). The dependency of domain patterns with stress and field history is investigated. Domain models explaining the observations will be discussed in detail. Funding through the DFG priority program SPP1239 is gratefully acknowledged.

MM 23.25 Tue 14:45 Poster B
Micromechanics of thin films of elastomeric polypropylenes — Mechtild Franke, Mario Zehn, Mario Jeczek, Robert Magele, and Nicolaus Reise — Chemische Physik, TU Chemnitz, 09107 Chemnitz
Elastomeric polypropylene consists of lamellar crystals embedded in an amorphous matrix. The arrangement, distribution, and connectivity of these crystals are important factors which determine the mechanical properties of the polymer. Free standing, ~1 µm thick films of different elastomeric polypropylenes are produced by dip coating the polymer solution on a NaCl crystal, floating the film onto water, and depositing it on a slotted silicon substrate. A stretching device, based on a piezoelastic drive, allows stretching the free standing film stepwise up to strains of 100%. The changes in shape, orientation, and morphology of crystalline regions are observed in situ with scanning force microscopy. Caused by the induced stress new lamellae crystallize; existing ones elongate or break into blocks. Furthermore, amorphous areas are stretched a lot more than crystalline ones. Volume images of thin films obtained with SFM based Nanotomography allow to explain some of the observed rearrangements of the microstructure.

MM 23.26 Tue 14:45 Poster B
Aktuelle Forschung an der Bonner Positronen Mikrosonde — Martin Heinze, Martina Wurtz, Patrick Eich, Matthias Haaks, and Karl Mair — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D-53115 Bonn
The Bonner Positronen Mikrosonde (BPM) is derzeit ein einzigartiges Messinstrument, das mit Hilfe der Positronenannihilation zerstörungsfrei die Defektdichte in Metallen und Halbleitern in hoher Ortsauflösung messen kann. Die BPM bietet einen fein fokussierten Positronenstrahl mit einzigartigem Stahlhuddurchmesser von 5 - 200 µm und ein integriertes Raster-
The Grain Refinement in a Commercial Al-Mg-Sc-Zr Alloy during Hot ECAP and Subsequent Isothermal Rolling — Olga Sukhopar1, Oleg Sidorov2,5, Günther Gottstein1, and Rustam Kakhshiyev4 — Institute of Physical Metallurgy and Metal Physics, RWTH, Aachen 52074, Germany

We perform molecular dynamics simulation with a recently developed new parameterisation of the embedded atom method (EAM) in order to investigate zinc nano-cluster. Nano-clusters exhibit differences in several properties compared to the bulk phase. In this context zinc is especially interesting because it is ahcp metal with a large deviation of the lattice axis ratio c/a to the ideal value corresponding to close packing. The clusters investigated here are obtained in prior particle formation simulations in a supersaturated vapour. The clusters are naturally potential energy minima, and their cluster isomerisation is controlled by the kinetic energy. In this contribution we have developed CNA signatures especially for hcp-surface structures that are important for particle growth. We also analyse the influences of the initial configuration to the resulting structures are not present. To control the temperature of the clusters we add argon as carrier gas which itself is coupled to a MD thermostat. We study the structure and morphology of the clusters for different temperatures and cluster sizes. Besides using the radial distribution function we employ the common neighbour analysis (CNA), which allows to determine details of the structural composition of the clusters. For this investigation we have developed CNA signatures especially for hcp-surfaces that are important for particle growth. We also analyse the thermal expansion and the equilibrium distance of the lattice constants for solid-like clusters.

MM 23.32 Tue 14:45 Poster B
Intershell conductance in multiwall carbon nanotubes — Andreas Stetter, Christian Back, and Johann Vanca — Universität Regensburg, Institut für angewandte Physik

We have measured the current induced voltage drop along an individual multiwall carbon nanotube (MWCNT) as a function of the distance to the current injecting electrode. For this purpose we used the scanning probe potential microscopy to determine the conductance of the MWCNT at different locations along the nanotube. To control the temperature of the clusters we add argon as carrier gas which itself is coupled to a MD thermostat. We study the structure and morphology of the clusters for different temperatures and cluster sizes. Besides using the radial distribution function we employ the common neighbour analysis (CNA), which allows to determine details of the structural composition of the clusters. For this investigation we have developed CNA signatures especially for hcp-surfaces that are important for particle growth. We also analyse the thermal expansion and the equilibrium distance of the lattice constants for solid-like clusters.

MM 23.34 Tue 14:45 Poster B
Fabrication of metallic nanowires and their hydrogen sorption — Felix Schlenkrich, Sonke Schmidt, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz
The influence of hydride formation on the resistivity of the wires was studied. Palladium wire alignments during hydrogen loading were performed in Non-Contact and Contact mode. Resistivity measurements on palladium wire alignments during hydrogen loading were performed. The influence of hydride formation on the resistivity of the wires will be discussed.

Quantum conductance of copper nanowires was investigated. The conductance of copper nanowires was measured using the self shadowing effect of the facets and ripples. Nanowire alignments of palladium and niobium have been produced. The behavior of metal wires during the exposure in hydrogen atmosphere was studied. Wire characterisation and the formation of metallic stripes onto the sample was achieved. Wire widths of 50nm and heights of 15nm were obtained. Silicon, using the self shadowing effect of the facets and ripples, was used. Nanowire alignments of palladium and niobium have been produced. The quantum conductance of copper nanowires was measured. The conductance of copper nanowires was measured using the self shadowing effect of the facets and ripples. Anomalous small-angle x-ray scattering was used to study the structural changes in complex materials which have coexisting inhomogeneities of different chemical composition. At different photon energies near an absorption edge, the scattering factor of the considered element changes significantly. By measuring at different photon energies near an absorption edge, the scattering factor of the considered element changes significantly. The dedicated instrument is optimized for this kind of measurement. The energy of the radiation can be tuned from 1 eV to 10 keV. At different photon energies near an absorption edge, the scattering factor of the considered element changes significantly. The dedicated instrument is optimized for this kind of measurement. The energy of the radiation can be tuned from 1 eV to 10 keV. The electrical properties of the nanowire were studied. Anodic oxidation has been used for formation of core-shell structures, protective layers, decorative or functional nanostructures. The first reaction product is found after 5 min thermal treatment at 110°C.
bon nanotubes (CNTs) are promising candidates for the integration into nanoelectromechanical systems such as nanorelays and actuators or transistors. Effective control of the CNT growth, orientation and positioning is still considered a major challenge within the scientific community.

In order to reach this goal, we use nanoparticles which are prepared via inert gas condensation as preformed catalysts to grow CNTs in thermal CVD and plasma enhanced CVD. Besides utilizing commonly used transition metal catalysts such as Fe, Ni and Co, we demonstrate the CNT growth from binary alloy catalyst particles, e.g. FePt.

**Phase diagrams for the evolution of polydomain and polyvariant states in tetragonal ferromagnetic martensites**  
- **Aristide T. Onisan¹, Nikolay S. Kiselev¹,², Ulrich K. Rössler¹, and Alexei N. Bogdanov¹,²,¹  
- IFW Dresden  
- Donetsk Institute for Physics and Technology

A continuum model for equilibrium microstructures in ferromagnetic twinned martensites is developed [1] that couples micromagnetic domain theory with anisotropic crystal elasticity and is applicable for magnetic shape memory materials as the Ni-Mn-Ga Heusler alloys. The approach considers the twin variant redistribution in tetragonal martensites with no-slip condition at the twin boundaries, magnetic 180°-domain structures within twins, and the rotation of magnetization within domains due to finite magnetic anisotropies. For two-variant twinned single crystals, we calculate equilibrium phase diagrams, strain and magnetization curves under combined external magnetic fields and stresses within the thermodynamic phase theory approximation. The limitations of the phase-theory approximation are discussed. For three-variant twinned microstructures, we show that the energy densities arise internally at the twin boundaries. A.N. Bogdanov, A. DeSimone, S. Müller, U.K. Rößler, J. Magn. Magn. Mater. 261 (2003) 204. Supported by DFG, SPP 1239 project A08.

**Correlated ferroelastic/ferromagnetic domain walls in ultrathin films: observations and physical description**  
- Catherine Jenkins¹,², R. Ramesh¹ and Gerhard Jakob²  
- ¹University of California, Berkeley  
- ²Johannes Gutenberg-Universität Mainz

The magnetic shape memory (MSM) effect is when simultaneously occurring ferromagnetic and ferroelastic domain walls form a twin boundary system that is actuated in one of three ways: by a magnetic field, a mechanical stress, or heating. Thin films of MSM alloys are exciting candidates for research because of the many variables that can be efficiently explored in a single system, and are promising for technological development for their novel magnetic and electronic characteristics.

Theoretical predictions in the literature (1), along with a physical understanding of the processes involved (2) together suggest that the thermoelastic austenite to martensite phase transition that allows for the ‘memory’ can be explored with temperature-dependent atomic force microscopy, as we show experimentally in fairly thick films of another shape memory alloy, nickel titanium. The behaviour of ultrathin films is expected to be noticeably different due to strong epitaxial clamping effects. In this work the expected topographic behaviour of ultrathin shape memory alloys during a magnetically and thermally induced phase transition and evolution is described and preliminary measurements presented.


**Laser ablation of aluminium**  
- Steffen Sonntag, Johannes Roth, Frank Gähler, and Hans-Rainer Trebin  
- Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

We investigate femtosecond laser ablation of metals using a hybrid simulation scheme. Two equations are solved simultaneously: one for the electronic system, which accounts for electron energy losses and heat conduction, the other for the dynamics of the lattice where the ablation process takes place. For the electron temperature a generalized heat conduction equation is solved by applying a finite difference scheme. For the lattice properties, e.g. pressure, density or temperature, we use common molecular dynamics. Energy transfer between the subsystems is allowed by introducing a phonon-phonon coupling term. This combined treatment of the electronic and atomic systems is an extension of the well known two-temperature model [1].

Atomic scale images of the ablation process are shown. The dependence of ablation and melting depth on characteristic parameters, such as the pulse duration and the laser fluence is discussed.


Phase change alloys are among the most promising materials for novel data storage devices. Among several classes of Phase Change Materials based on Ge-Sb-Te alloys have been used in optical data storage solutions like rewritable CDs and DVDs. Recently these alloys have been explored as potential candidates for fast nonvolatile electrical data storage devices. Since several years Phase Change Materials are among the most promising materials for novel data storage devices. Since several years Phase Change Materials.

Aachen — 2

Phase change alloys are among the most promising materials for novel data storage devices. Among several classes of Phase Change Materials based on Ge-Sb-Te alloys have been used in optical data storage solutions like rewritable CDs and DVDs. Recently these alloys have been explored as potential candidates for fast nonvolatile electrical data storage devices. Since several years Phase Change Materials are among the most promising materials for novel data storage devices. Since several years Phase Change Materials.

MM 23.48 Tue 14:45 Poster B
Crystallography of phase change materials — ANDREAS KALDENBACH, MARTIN SALINGA, URSULA NELLEN, CARL SCHLOCHER-MAIN and JENNIFER LUCKAS — 1. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase Change RAM is one of the most promising technologies for future memory applications outperforming alternatives mainly by its extreme scalability besides its non-volatility. It is based on a so-called phase change material switching between its highly resistive amorphous and lowly resistive crystalline state. While phase change materials are already utilized in applications, their remarkable physical properties and their potential for rapid melting of pure metals — D. M. Herlach, D. M. Herlach, D. M. Herlach.

Besides attracting considerable interest from the commercial point of view phase change materials are very interesting also due to their remarkable physical properties. They have the ability to be reversibly switched within a few nanoseconds between the amorphous and the crystalline phase, while changing their physical properties such as optical reflectivity and electrical resistivity significantly. Even though the electronic properties show a drastic contrast such fast transitions can only be caused by small atomic rearrangements. This behavior calls for a deeper understanding of the structural properties of the alloys.

We have performed powder diffraction measurements of the crystal phase of various GeSbTe alloys, to determine the structural similarities and differences of several alloys. Understanding the crystal structure of phase change materials is a key to a deeper insight into the properties of these promising materials.

MM 23.49 Tue 14:45 Poster B
Characterization of a FePd single crystal for sensor applications — CHRISTOPH BARCHI1, ANDREAS GEHRER1, MANFRED WUTTIG2, ECKHARD QUANDT3, JEFF MCCORD4, YIU WAI LAI4, JÖRG BUSCHEM5, LUDWIG SCHULTZ2, OLEG HECZKO1, and SEBASTIAN FAHLEN1 — 1. Research Center caesar, Ludwig-Erhard-Allee 2, 53719 Bad Honnef — 2. Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 — 3. Christian-Albrechts-Universität zu Kiel, Chair for Inorganic Functional Materials, Kaiserstr. 2, 24143 Kiel — 4. IFW Dresden, P.O. Box 270166, 01171 Dresden

Magnetostrictive materials have a prime role in magnetic data storage. In recent years, the demand for high-density magnetic recording has led to a new type of magnetic recording, namely perpendicular magnetic recording. Perpendicular recording allows for higher areal densities than the traditional in-plane magnetic recording, which is currently used in hard disk drives. In order to achieve high recording densities, perpendicular magnetic recording requires materials that exhibit large magnetic anisotropy and high coercivity.

MM 23.50 Tue 14:45 Poster B
Molecular dynamics simulation study of crystal growth and melting of pure metals — ROBERTO ROZAS and JUERGEN HORSTJES — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linden Höhe, 51147 Köln

The crystallization of Ni is studied by non-equilibrium molecular dynamics simulation. Interactions between atoms are described by a potential of the embedded atom type (EAM). As an initial configuration particles are placed in an elongated simulation box where the crystalline fcc phase in the middle is surrounded by the undercooled liquid phase, separated by two interfaces. The temperature dependence of the interfacial growth is determined by two methods: (i) a global method based on the evolution of the density, (ii) a local method based on a common neighbor analysis and the cone algorithm. The three crystal orientations (100), (110) and (111) are considered. Effects associated with technical aspects of the simulation, such as the influence of thermostat and barostat on crystal growth, are also investigated.

MM 23.51 Tue 14:45 Poster B
USAXS measurements of undercooled charged colloidal model systems — INA KLASSEN1, PATRICK WUTTIG2, DIRK HOLLAND-MORITZ1, DIETER M. HERLACH1, THOMAS PALBERG1, and STEPHAN V. ROTH1 — 1. Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linden Höhe, 51147 Köln, Germany

We analyzed a colloidal system of charged silica particles in aqueous dispersion. The crystallization of charged colloids is driven by strong long-range electrostatic interactions between the particles. The main parameter governing the interaction is the surface charge number of the particles which can be varied in a controlled way by addition of sodium hydroxide.

Our system is characterized by convenient time scales of seconds and particle distances of microns and thus accessible by simple, yet powerful optical techniques. Microscopy and light scattering yield complementary information on equilibrium properties and crystallization kinetics from real and reciprocal space (phase behaviour, solidification mechanisms, growth velocities, nucleation rate densities). With these results we can determine the degree of undercooling of our system. Structural changes of the melt with increased undercooling and the corresponding changes of the solidification can be monitored by Ultra Small Angle X-Ray Scattering (USAXS) performed at Hasylab (Hamburg).

MM 23.52 Tue 14:45 Poster B
Elasticity and solidification kinetics in a eutectic-like two component colloidal system — INA J. LORENZ and THOMAS PALBERG — Institute of Physics, University of Mainz, Germany

Colloidal systems of charged spherical particles in deionized aqueous suspension show a first order phase transition to a crystalline state (bcc or fcc) once the strength and range of the screened Coulomb repulsion are sufficiently large. Recently we also investigated the phase behaviour of binary charged mixtures using static light scattering, to find random composition bcc crystals at charge and size ratios close to one, the onset of compound formation at ratios below 0.7 and a eutectic-like phase behaviour at ratios around 0.55 with strong indications of a gravitational assisted demixing [1]. The kinetics of the latter mixture was monitored via the evolution of the shear elasticity employing torsional resonance spectroscopy. While the pure components and the mixtures far from the eutectic composition solidify via homogeneous nucleation within a few minutes, closer to the eutectic composition the shear modulus of the mixtures is significantly lower. The system is finally solidified when the completely solidified state. We discuss the coupling of crystallization kinetics to the kinetics of demixing, which depend on both the composition and the ‘undercooling’ which for our systems is approximately linear in particle concentration.