# 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[1], Christian Zeitz[2], Christian Dietz[1], Nadine Drechsel[1], Anke Bernstein[3], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken — [3]Experimentelle 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 length scale these materials have a stiff inorganic component (hydroxylapatite) 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 in-situ in the 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[1], Michael Horisberger[2], Thomas Gutberlet[2], Jochen Stahn[2], and Harald Schmidt[1] — [1]Institut für Metallurgie, AG Materialphysik, TU Clausthal, Germany — [2]Laboratorium 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 nanocrystalline Fe films using neutron reflectometry. This method enables to determine extremely low diffusivities down to 10ˆ-25 mˆ2/s and also extremely small diffusion lengths < 1 nm, not possible with conventional methods. For diffusion studies, isotopic multilayers of the form Si(substrate)/[57-Fe(5 nm)/nat-Fe(10 nm)]x10 were deposited by using magnetron sputtering. The multilayers were annealed in the temperature range between 473 and 673K for different periods of time and neutron reflectivity has been measured in-situ. Further, structural characterization has been done by grazing incidence X-ray diffractometry, Moessbauer spectroscopy, atomic force microscopy, and electron microscopy. First results are presented and are discussed in the framework of grain boundary diffusion in the type C regime.

MM 23.3 Tue 14:45 Poster B

**Nitrogen Diffusion in Amorphous Silicon (Carbo)Nitride Probed by Neutron Reflectometry** — •Erwin Hüger[1], Thomas Gutberlet[2], Jochen Stahn[2], Michael Bruns[3], and Harald Schmidt[1] — [1]Institut für Metallurgie, AG Materialphysik, TU Clausthal, Germany — [2]Laboratorium für Neutronstreuung, ETH Zuerich & PSI, Villigen, Switzerland — [3]Institut für Materialforschung III, Forschungszentrum Karlsruhe GmbH, Germany

Covalently bound amorphous solids are distinguished by extremely low self-diffusivities, which necessitates the detection of extremely short diffusion lengths in order to prevent an overlapping of crystallization and diffusion processes during annealing. We present nitrogen diffusion studies on amorphous $SiN_x$ and $SiC_xN_y$ materials, which were carried out by neutron reflectometry on isotope heterostructures. Here, a sequence of 14-N and 15-N enriched layers are deposited by magnetron sputtering on silicon substrates. Due to the different coherent neutron scattering lengths of 14-N (9.37 fm) and 15-N (6.44 fm) a scattering contrast for neutrons occurs between chemically identical layers. Self-diffusivities are determined from the modification of the reflectivity due to interdiffusion of the two nitrogen isotopes after annealing at elevated temperatures. We present a systematic study on samples with 3, 5, 12 and 40 single layers and demonstrate that it is possible to detect miniumum diffusion lengths of 0.7 nm and self-diffusivities of $5x10^{-25} m^2/s$. The temperature and annealing time dependence of the diffusivities is analyzed and explained in the framework of structural relaxation processes.

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 Sternemann[1], Christian Sternemann[1], John S. Tse[2], Juha A. Soininen[3], Yong Q. Cai[4], Serge Desgreniers[5], Timothy T. Fister[6], Nozomu Hiraoka[4], Achim Hohl[7], Andreas Schacht[1], Gerald T. Seidler[6], György Vankó[8,9], Simo Huotari[8], Keijo Hämäläinen[3], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, TU Dortmund, Germany — [2]Dept. Phys. & Engn. Phys., U Saskatchewan, Canada — [3]Div. X-ray Phys., Dept. Phys. Sci., U Helsinki, Finland — [4]NSRRC, Hsinchu, Taiwan — [5]Dept. Phys., U Ottawa, Canada — [6]Phys. Dept, U Washington, USA — [7]Inst. Mat. Sci., TU Darmstadt, Germany — [8]ESRF, Grenoble, France — [9]KFKI, Budapest, Hungary

Non-resonant inelastic x-ray scattering is a powerful tool to access shallow absorption edges using hard x-rays. This allows the study of low energy transitions under conditions which do not permit electrons and soft x rays as a probe. We present a variety of non-resonant inelastic x-ray scattering measurements of Si based compounds. Applications range from L-edge studies of elemental Si [1] and bulk amorphous Si monoxide [2] to the study of giant dipole resonances of Ba and I endohedrally intercalated in complex silicon networks. The experimental results are compared to calculations employing a real-space multiple-scattering approach [3]. Implications on the study of high-pressure induced phase transitions will be emphasized.

[1] H. Sternemann *et al.*, Phys. Rev. B **75**, 075118 (2007). [2] C. Sternemann *et al.*, J. Phys. Chem. Solids **66**, 2277 (2005). [3] J.A. Soininen *et al.*, Phys. Rev. B **72**, 045136 (2005).

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[1], Rossitza Pentcheva[1], and Jim Rustad[2] — [1]Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — [2]Department 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 oxyhydroxide-polymorphs ($\alpha$-, $\beta$-, $\gamma$- and *hp*-FeOOH) under high pressures. We find that under ambient conditions goethite ($\alpha$) 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

(GGA). However, a substantial improvement of the size of the band gap is achieved by including electronic correlations within the LDA+U method.
[1] C. Laberty and A. Navrotsky, Geochimica et Cosmochimica Acta 62, 2905-2913 (1998)

MM 23.7 Tue 14:45 Poster B

**Investigation of Electronic Transport Mechanisms in Phase Change Materials** — •Jennifer Luckas, Martin Salinga, Carl Schlockermann, Andreas Kaldenbach, Ursula Nellen, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

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 validate or disprove them. To fill this gap in this work the mobility of the charge carriers is studied for some representative phase change materials. The dependence of the mobility both 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.

MM 23.8 Tue 14:45 Poster B

**High Kinetic Energy Photoelectron Spectroscopy Study of the Ni 1s Core Level and Satellite Structure** — •Mihaela Gorgoi[1], Svante Svensson[2], Olof Karis[2], Jan Rusz[2], Peter Oppeneer[2], Franz Schäfers[1], Walter Braun[1], Nils Martensson[2], and Wolfgang Eberhardt[1] — [1]BESSY GmbH, Berlin, Germany — [2]Uppsala 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 satellite problem and requires a revision of current models.

[1] A.P. Grosvenor, M.C. Biesinger, R.St.C. Smart, N.S. McIntyre, Surface Science 600 (2006) 1771.

[2] A. Bosch, H. Feil, G.A. Sawatzky, N. Mårtensson, Solid State Communications 41 (1982) 355.

MM 23.9 Tue 14:45 Poster B

**The importance of cluster-distortions in the tetrahedral cluster compounds: Ab initio investigations** — Martin Sieberer, Stefan Turnovszky, Peter Mohn, and •Josef Redinger — Center for Computational Materials Science, Vienna University of Technology, Vienna, Austria

We study the electronic and structural properties of selected representatives of the so-called Molybdenum cluster compounds such as $GaM_4X_8$ with M=Mo as a group VIB element and V, Nb, Ta as a group VB element. X denotes either S or Se. These compounds are known to exhibit semiconducting behavior in the electrical resistivity, caused by hopping of electrons between well-separated metal clusters. The large separation of the tetrahedral metal ($M_4$) clusters is believed to be the origin of strong correlations. We show that recent calculations neglected an important type of structural distortions, namely those happening only within the $M_4$ unit upon a fixed angle $\phi = 60^o$ of the trigonal (fcc-like) cell. These internal distortions gain a significant amount of energy compared to the cubic cell and they are - to our knowledge - almost undetectable within powder x-ray diffraction. However, they strongly influence the band-structure by opening up a gap at the Fermi-energy, which puts into question whether all compounds of this family are really called Mott insulators as stated elsewhere. In particular ferromagnetic $GaMo_4S_8$ and $GaV_4S_8$ are well described within DFT. Only the Nb and Ta-based representatives require a large effort due to the lack of magnetic long range order caused by frustrated AF M-M interactions.

MM 23.10 Tue 14:45 Poster B

**Critical Packing Fraction in Multicomponent, Glass Forming Metallic Liquids** — •Suresh M. Chathoth, 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 quasielastic 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.

1.S. Mukherjee, Z. Zhou, W. L. Johnson, and W. K. Rhim, J. Non-Cryst. Solid 337, 21 (2004).

2.W. Götze, J. Phys: Condens. Matter 2, 8485 (1990).

MM 23.11 Tue 14:45 Poster B

**Temperature dependence of elastic constants for the metallic glass $Pd_{40}Ni_{40}P_{20}$** — •Thomas Koeppe, Dennis Bedorf, and Konrad Samwer — 1. Physikalisches Institut Universität Göttingen, Germany

We have measured the elastic constants of bulk amorphous $Pd_{40}Ni_{40}P_{20}$ 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 decreasing temperature and deviates from that behavior at low temperatures also. This behavior is qualitatively the same as for single crystals and follows a $T^{\frac{3}{2}}$ - 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.

MM 23.12 Tue 14:45 Poster B

**Influence of a miscut of $Y_2O_3$-stabilized $ZrO_2$ single crystals on the formation of $La_2Zr_2O_7$ islands by a vapour-solid reaction** — •Markus Andreas Schubert, Stephan Senz, and Dietrich Hesse — Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The $La_2Zr_2O_7$-forming solid state reaction between $ZrO_2$ and $La_2O_3$ is of significance in view of solid oxide fuel cells degrading during operation by a reaction of this type, if $ZrO_2$ is the solid electrolyte and if a $La_2O_3$-containing ternary oxide cathode is used. In model experiments, $La_2O_3$ vapour at 1200 °C directly reacts with an yttria-stabilized $ZrO_2$ single crystal (YSZ) forming $La_2Zr_2O_7$ (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 $[\bar{1}10]$ 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 $[\bar{1}10]$ or [001] direction. The relative orientation and morphology of the LZO islands were investigated by AFM, XRD and TEM.

MM 23.13 Tue 14:45 Poster B

**PAC studies of Indium containing MAX phases** — •Daniel Jürgens[1], Michael Uhrmacher[1], Hans Hofsäss[1], Jens Röder[2], Pawel Wodniecki[3], Agniszka Kulinska[3], and Michel Barsoum[4] — [1]II. Physik. Inst., Universität Göttingen, Germany — [2]Institut f. phys. Chemie, TU Braunschweig,Germany — [3]IFJPAN, 31 - 342

Krakow, Poland — [4]Dep. Mat. Science and Eng. Drexel Univ., Philadelphia, USA

Nanolaminated layered ternary carbides and nitrides, the so called MAX phases, have attracted great attention in recent time. By now over 50 compounds are known which feature a unique combination of the best attributes of both metals and high-performance ceramics. 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 $Ti_2InC$ and $Zr_2InC$. 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** — •Mira Sakaliyska, Kumar Babu Surreddi, Sergio Scudino, and Jürgen Eckert — IFW Dresden, Institut für Komplexe Materialien, Postfach 270116, 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-Al3Mg2 and gamma-Al12Mg17) during milling was detected. Similar results can be achieved by mechanical milling of intermetallic compounds. For example, for Al60Mg40 mechanical alloying and milling yield the same metastable supersatured 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 increasing temperature. At higher temperature, a hexagonal phase with composition Al3Mg2, is formed. The subsequent exothermic events correspond to formation and growth of the equilibrium beta-Al3Mg2 phase. Finally, selected examples for the mechanical deformation behavior of consolidated samples are presented, revealing encouraging properties regarding the combination of high strength and good ductility at room temperature.

MM 23.15 Tue 14:45 Poster B

**New DFT-Investigations of Vanadium Silicides** — Mike Thieme and •Sibylle Gemming — 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 band-structure 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 determined. 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 pressure** — •Claudia Loose[1], Jens Kortus[1], Marcus Schwarz[2], Edwin Kroke[2], and Gerhard Heide[3] — [1]TU-Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany — [2]TU-Bergakademie Freiberg, Institute for Mineralogy Brennhausgasse 14 09596 Freiberg, Germany — [3]TU-Bergakademie Freiberg, Institute for Anorganic Chemistry, Leipziger Straße 29, Germany

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 $V_0$ at different pressure ranges. We also calculated transition pressures for the system ALN (wurtzite - rocksalt) and $SiO_2$ (low quarz - coesite - stishovite) with respect to Pseudopotential and EOS. At low pressure all EOS gave similar elastic properties whereas encreasing 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 choise of Pseudopotential (LDA/GGA)

MM 23.17 Tue 14:45 Poster B

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

Electrochemical capacitors (EC) fill the gap between conventional capacitors 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 electrostatically in the electrochemical double-layer between electrolyte and high surface area electrodes of activated hard carbon. In pseudocapacitance supercapacitors the charge storage is of faradaic-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 the faradaic- and the double-layer capacitance of the metal oxide and carbon, respectively, to increase the achievable capacity of the electrode. The electrochemical properties of these composites were investigated with cycling voltammetry, charge/discharge cycling and impedance spectroscopy. Structural analysis was performed via scanning electron microscopy and X-ray diffraction.

MM 23.18 Tue 14:45 Poster B

**The Imaging Beamline at PETRA III** — •Astrid Haibel, 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 brillance (most brilliant X-ray source worldwide), the low emittance of 1nm rad (unrivaled for current storage rings at comparable high particle energies) and the high fraction of coherent 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 fulfil 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 stations for micro and for nano tomography. The X-ray energy will be tunable between 5 and 50 keV. In the micro tomography hutch the investigation 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 (SR$\mu$CT) and neutron tomography (NCT) for materials science** — •Felix Beckmann, Julia Herzen, Tilman Donath, Astrid Haibel, Thomas Dose, Jürgen Vollbrandt, Heinz-Werner Schmitz, Philipp Klaus Pranzas, 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 storage ring DORIS 3 at DESY Hamburg. In the recents years 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 microtomography at HARWI II and new enhancements and applications using lower photon energies at the wiggler beamline BW2 will be presented. Furthermore at the research reactor FRG-1 the neutron radiography facility GENRA 3 was extended by a setup for neutron tomography. Results performing SR$\mu$CT 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** — •Horst Katterwe — Kriminaltechnisches Insitut / 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 are 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, Simross "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** — •Jürgen Gegner — 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. Fick'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 study, and realistic prediction, SimCarb 2006 allows for efficient 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** — •Torben Fischer, René V. Martins, and Andreas Schreyer — GKSS research centre, Max-Planck-Str. 1, 21502 Geesthacht

In civil aircraft production advanced welding techniques, like laser beam 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 influence on the service performance of the weld. For strain scanning GKSS research centre built up the high energy materials science beamline HARWI II at HASYLAB. The use of high energetic photons from about 80keV - 120keV enables diffraction experiments in transmission geometry, which provides the information about the macroscopic stresses. A large sample-detector-distance ensures 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 influences of the gauge volume size and grain statistics on the strain measurements were systematically investigated. For the t-joint configuration two dimensional stress maps were calculated from the data. For the near future an in-situ FSW experiment is planed 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[1,2], Igor E. Dragunov[2], Aristide T. Onisan[1], •Ulrich K. Rössler[1], and Alexei N. Bogdanov[1,2] — [1]IFW Dresden — [2]Donetsk Institute for Physics and Technology

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.

[1] Y. W. Lai et al., Appl. Phys. Lett. 90 (2007) 192504; [2] V. A. Chernenko et al., Acta Mater. 53 (2006) 5461. [3] N. S. Kiselev et al., Eur. Phys. J. Special Topics, to appear.

MM 23.24 Tue 14:45 Poster B

**Dependency of magnetic domain structures on stress and field history in bulk NiMnGa** — •Ryan Yiu Wai Lai, Jeffrey McCord, Rudolf 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** — •Mechthild Franke, Mario Zerson, Mario Jecke, Robert Magerle, and Nicolaus Rehse — 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, $\sim$1 $\mu$m 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 piezoelectric 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** — •Sven-Martin Hühne, Marius Wirtz, Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D - 53115 Bonn

Die Bonner Positronen Mikrosonde (BPM) ist 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 einstellbarem Stahldurchmesser von 5 - 200 $\mu$m und ein integriertes Raster-

elektronenmikroskop (REM). Dadurch ist es möglich mit der BPM mit hoher lateraler Auflösung Plastizität und Defektdichte in verschiedenen Materialien zu messen.

Aktuelle Forschungsschwerpunkte liegen in der Abbildung von Deformationszonen und Ermüdungsstrukturen. Des Weiteren werden die Ergebnisse der durch Positronenannihilation gemessenen Defektdichte mit den klassischen Methoden zur Bestimmung der Schädigung wie Röntgen-Beugung (Debye-Scherrer Methode) und Vickers-Härte Messungen verglichen. Die in den Abbildungen erkennbare Entwicklung der Fehlstellendichte wird zur Vorhersage des Materialversagens in der Deformationszone herangezogen. Es zeigt sich, dass die Untersuchung der Defektdichte zu einer präzisen Schadensvorhersage führt, wie sich an aktuellen Messungen von Ermüdungsstrukturen an ferritischem und austenistischem Stahl veranschaulicht hat.

MM 23.27 Tue 14:45 Poster B

**Introduction of Slip System Resolved Statistical Work Hardening Model** — •Denis Novokshanov and Volker Mohles — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen Kopernikusstr. 14, D-52074 Aachen, Germany

A slip system resolved statistical work hardening model for single crystals has been developed. It is based on the dislocation density-based work hardening model 3IVM+, which in turn is an improved version of the 3IVM (three internal variables model) [1]. 3IVM+ predicts stress-strain curves for large ranges of temperature and strain rate. In the new model, the microstructure evolution of 3IVM+, i.e. the dislocation density evolution, is left unchanged. But the kinetic equation of state of 3IVM+ has been inverted: the new model considers the glide velocity of dislocations as a function of temperature and the external applied stress. This allows to consider each glide system individually by applying the corresponding Schmid factor in the stress projection. Hence all slip systems contribute to the overall deformation according to their intrinsic kinetics, which is defined by the crystal's orientation and the load axis. This leads tho realistic stress-strain curves and orientation changes for a single crystal. The model can be used as a replacement for 3IVM(+) in engineering applications of FEM. For polycrystals, the interaction between grains can be introduced in future by elastic stresses caused by differing rotations of adjacent grains.

1. F. Roters, D. Raabe, G. Gottstein, Acta Materiallia 48 (2000) 4181-4189

MM 23.28 Tue 14:45 Poster B

**$Pd_{81}Si_{19}$-Metallic Nanoglasses with Enhanced Excess Volume** — •Yue Zhang, Horst Hahn, and Herbert Gleiter — Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

$Pd_{81}Si_{19}$ metallic nanoglasses were synthesized by inert gas condensation and in situ compaction. In this technique, amorphous nanoparticles, prepared by evaporation in an inert gas atmosphere, are collected and subsequently compacted using uniaxial pressures. During the compaction, surfaces are converted into internal interfaces and additional free volume is introduced into the amorphous structure. Wide angle X-ray diffraction and high resolution electron microscopy are employed to characterize the atomic structure. The excess volume fraction was calculated using classical free-volume theory from differential calorimetric scanning data. In order to have a comparison, glassy ribbons and bulk metallic glass rods with the same chemical composition were prepared using melt-spinning and $B_2O_3$ flux casting techniques, respectively. Comparing with these conventional metallic glasses, the $Pd_{81}Si_{19}$ nanoglasses exhibit an enhanced excess volume, resulting in modified properties.

MM 23.29 Tue 14:45 Poster B

**The Grain Refinement in a Commercial Al-Mg-Sc-Zr Alloy during Hot ECAP and Subsequent Isothermal Rolling** — •Olga Sukhopar[1], Oleg Sitdikov[2,3], Günter Gottstein[1], and Rustam Kaibyshev[4] — [1]Institute of Physical Metallurgy and Metal Physics, RWTH, Aachen 52074, Germany — [2]Institute for Metals Superplasticity Problems, Ufa 450001, Russia — [3]Department of Engineering Physics, Electronics and Technology, Nagoya Institute of Technology, Nagoya 466-855, Japan — [4]Belgorod State University, Belgorod 308034, Russia

Grain refinement taking place in a commercial Al-Mg-Sc-Zr alloy under equal channel angular pressing (ECAP) and subsequent isothermal rolling, which were carried out at a temperature of 325°C, was examined. With increase of strain the initial grains were highly elongated along the extrusion direction, and new fine grains formed along initial boundaries composing mantle region. Then new grains with size ~ 1.5 $\mu$m were evolved in the grain interiors. During subsequent rolling the fraction of recrystallized grains increases. However, even after highest strains attained no full recrystallized structure was observed. Texture measurements have shown a randomly oriented structure. These results suggest that the dynamic evolution of new grains can be result from (sub)grains rotation, which leads to a rapid increase in misorientation of grain boundaries and to texture randomization. It was shown that progressive increase of misorientation of deformation induced boundaries (continuous dynamic recrystallization) is the main mechanism of submicrocrystalline grain formation.

MM 23.30 Tue 14:45 Poster B

**zinc nano-cluster investigated by molecular dynamic simulations** — •Stephan Braun, Frank Römer, and Thomas Kraska — Institute for Physical Chemistry, University Cologne, 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 a hcp 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 grown including cluster-cluster collisions and sintering. 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 23.31 Tue 14:45 Poster B

**Wassersorption in porösen Kohlenstoffen** — •Philipp Eitelwein, Stephan Braxmeier und Gudrun Reichenauer — Bayerisches Zentrum für Angewandte Energieforschung, Am Hubland, 97074 Würzburg

Wird Wasserdampf in porösen Kohlenstoffen adsorbiert, so lässt sich eine makroskopische Längenänderung der Probe feststellen. Diese Änderung hängt vom relativen Druck des umgebenden Wasserdampfs ab. Es zeigt sich außerdem, dass sich die Adsorption in Poren unterschiedlicher Größe unterschiedlich verhält, denn Mikroporen (Poren $< 2$ nm) lassen sich über Adsorption aus der Gasphase vollständig befüllen, während dies bei Meso- und Makroporen nicht der Fall ist. Zum besseren Verständnis wurden systematische Untersuchungen an Kohlenstoff-Aerogelen als Modellmaterial durchgeführt. Diese synthetischen Kohlenstoffe besitzen sowohl Makro- oder Mesoporen als auch Mikroporen; beide Spezies können während der Synthese gezielt variiert werden. Mittels unterschiedlicher Methoden, wie Röntgenkleinwinkelstreuung an unterschiedlich stark befeuchteten Proben und Messung von Sorptionsisothermen bei gleichzeitiger Bestimmung der Probenlänge, wird der Einfluss der Porengrößen auf die Längenänderung der Probe bei Ad- und Desorption systematisch untersucht. Aus den Daten werden Rückschlüsse auf die mit der Sorption auf mikroskopischer Längenskala verknüpften Effekte gezogen.

MM 23.32 Tue 14:45 Poster B

**Intershell conductance in multiwall carbon nanotubes** — •Andreas Stetter, Christian Back, and Johann Vancea — Universität Regensburg, Institut für angewandte Physik

We have measured the current induced voltage drop along an individual mutiwall carbon nanotube (MWCNT) as a function of the distance to the current injecting electrode. For this purpose we used the scanning probe potentiometry combined with scanning electron microscopy.

For a MWCNT with an incomplete outer shell a sharp potential jump was observed at the end of the outer shell. The length dependence of the potential on the whole tube has been used to determine the intershell conductance of the MWCNT.

MM 23.33 Tue 14:45 Poster B

**Fabrication of metallic nanowires and their hydrogen sorption** — •Felix Schlenkrich, Sönke Schmidt, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz

1, 37077 Göttingen

Nanowire alignments of palladium and niobium have been produced by small angle sputtering onto facetted sapphire and sputter-eroded silicon, using the self shadowing effect of the facets and ripples, respectively. The achieved wire length is in the cm range (length of sample) and wire widths of 50nm and heights of 15nm were obtained. Island growth has been investigated, and the regimes of coalescence and fully covered wire morphology of the metallic stripes onto the facets and ripples were achieved. Wire characterisation and the behaviour of metal wires during the exposure in hydrogen atmosphere (surface modification) was investigated with STM and AFM, using Non-Contact mode 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.

MM 23.34 Tue 14:45 Poster B

**Quantum conductance of copper nanowires** — •Saeideh Mohammadzadeh[1], Davoud Pouladsaz[2], Reinhard Streiter[1], and Thomas Gessner[1] — [1]Zentrum für Mikrotechnologien, Technische Universität Chemnitz — [2]Institut für Physik, Technische Universität Chemnitz

Electronic transport properties of the Cu nanowires are studied using theoretical analysis based on non-equilibrium Green function's technique within the density functional tight-binding method. The systems, presented in this work, consist of Cu nanowires in various crystalline directions, coupled between semi-infinite copper electrodes. The current-voltage characteristics of the wires and charge density with non-equilibrium conditions are investigated as well.

MM 23.35 Tue 14:45 Poster B

**Determination of lattice distortion in nanoparticles on strained substrates using molecular dynamics** — Jian Zhou, •Srinivasa Saranu, and Ulrich Herr — Institut für Mikro- und Nanomaterialien, Universität Ulm, 89081 Ulm

Magnetoelastic anisotropies might provide a way to optimize the magnetic properties of nanoparticles. The experimental determination of strain in nanoparticles is often complicated by the low XRD intensities. We used the molecular dynamics simulation technique to determine the deformation of Co particles deposited on Ta or Cu substrates. Co particles of 4.5 nm diameter with fcc structure were built using a Wulff construction and subsequently deposited on the substrates with a kinetic energy of 0.1eV/atom. The structure and internal strain in the particles have been determined from simulated diffraction curves. In some cases we find a fcc-to-hcp phase transformation in the particles which turns out to be related to the impact energy and the interface structure between the particle and substrate. The analysis also shows that the landed particles are always tilted with respect to the substrate surface. The degree of tilt is associated with the shape of the Co Wulff polyhedron. We have also studied the deformation induced in the particles by a change of the lattice parameter of the substrate after the deposition. We find that only coherent or semicoherent interfaces can transfer strain from the substrate to the deposited Co particles effectively.

MM 23.36 Tue 14:45 Poster B

**Anomalous small-angle x-ray scattering beamline B1 at HASYLAB, DESY** — •Ulla Vainio[1], Günter Goerigk[2], and Rainer Gehrke[1] — [1]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Postfach 1913, D-52425 Jülich, Germany

Anomalous small-angle x-ray scattering (ASAXS) is a contrast variation technique used for studying the structure of complex materials which have coexisting inhomogeneities of different chemical composition. By measuring at different photon energies near an absorption edge of a certain chemical element contained in the sample, the small-angle scattering caused by the distribution of that element can be distinguished from other scattering contributions caused by other elements or by voids in the case of porosity. This is possible because the scattering factor of the considered element changes significantly near its absorption edge.

The dedicated instrument is optimized for this kind of measurement in terms of precision. The energy of the radiation can be tuned from 5 keV up to 35 keV and accurate x-ray absorption scans can be performed.

The beamline is located at a bending magnet at the DORIS storage ring. It was originally built by research centre Jülich in the 1980s and was upgraded in collaboration with HASYLAB in 2006 (G. Goerigk (2006) HASYLAB annual report, pp. 77 - 78) . Since July 2007 the beamline is operated by HASYLAB.

MM 23.37 Tue 14:45 Poster B

**Stress impact on reactive diffusion in nano-structures of spherical symmetry** — •Constantin Buzau Ene[1], Guido Schmitz[2], Carsten Nowak[1], Talaat Al-Kassab[1], and Reiner Kirchheim[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund Platz 1, D-37077 Göttingen — [2]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str.10, D-48149 Münster

Al/Cu/Al and Cu/Al/Cu triple layers with approximately 10 nm single layer thickness are deposited on curved substrates of 25 nm radius and investigated by atom probe tomography. The first reaction product is found after 5 min thermal treatment at 110°C. Surprisingly, the reaction rate depends significantly on the deposition sequence of the metals. Thus, the thickness of the product formed at the interfaces at which Cu is deposited on top of Al is approximately 1.5 to 2 times thicker than that of the opposite stacking sequence. This asymmetry may be explained by stress induced by excess volume of the reaction product. Due to the specific geometry, compressive and dilatational stress is produced on opposite sides of the product layer, even in the case of semi-coherent or incoherent interphase boundaries. The resulting stress gradient leads to additional driving force to the transport of vacancies which accelerates or decelerates the reaction rate in dependence on the stacking sequence of the layer material. By quantitative analysis, the level of induced stress can be quantified from the modified growth rates.

MM 23.38 Tue 14:45 Poster B

**Charge separation between type II aligned closed packed CdTe and CdSe nanocrystals** — •Dieter Gross, Andrei S. Susha, Thomas A. Klar, Andrey L. Rogach, and Jochen Feldmann — Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Germany

Combinations of CdTe and CdSe provide type II structures with the lowest excited energy state for electrons in CdSe and the lowest excited hole state in CdTe. This kind of energy level alignment facilitates the separation of photo-excited charge carriers in modern thin film solar cells. We have observed an efficient photoluminescence quenching and a reduced life time of the CdTe nanocrystal emission in hybrid structures made of colloidal CdTe and CdSe nanocrystals. These effects have been observed in both, layered structures created by a layer-by-layer technique and clustered assemblies in solution, providing both a controlled assembly with a short inter-particle distance ($< 1$ nm). We interpret this suppression of the CdTe emission to be due to spatial charge separation of the photo-excited electron-hole pairs.

MM 23.39 Tue 14:45 Poster B

**Tailoring the diameter of nanowires by controlled anodic oxidation and its electrical properties** — •Seid Jebril, Samia Essa, Mady Elbahri, and Rainer Adelung — Functional Nanomaterials, Institute for Material Science, CAU Kiel, Kaiserstr. 2, 24143 Kiel

Resizing the diameter of the already formed nanowire has been a great challenge to achieve for the last decades. Here, we show tailoring of a nanowire by using anodic oxidation. Anodic oxidation has been used for formation of core-shell structures, protective layers, decorative or functional properties, to cite some. The polycrystalline nanowire used in this experiment was made by a method similar to what we developed earlier [1, 2]. We studied the electrical properties of the nanowire during and after the process. As a result of this potential controlled anodic oxidation, the diameter of the nanowire gets smaller and smaller as the oxide grows. Therefore, the electrons encounter dominant surface and boundary scattering due to confinement. Hence, the electronic properties change completely.

[1] R. Adelung et. al., Nature Mater. 3, 375, (2004).
[2] M. Elbahri et al., Adv. Mater. 18, 1059 (2006).

MM 23.40 Tue 14:45 Poster B

**Tailoring carbon nanotubes through predefined catalyst particles** — •Christoph Schünemann, Franziska Schäffel, Mark H. Rümmeli, Christian Kramberger, Thomas Pichler, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Owing to their excellent mechanical and electronic properties, car-

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 mayor challenge within the scientific community.

In order to reach this goal, we use nanoparticles which are prepared via inert gas condensation as predefined 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.

MM 23.41 Tue 14:45 Poster B

**Electric field controlled metal-oxide transformation of metal nanowires** — •Carsten Nowak[1], Guido Schmitz[2], and Reiner Kirchheim[1] — [1]Universität Göttingen, Institut für Materialphysik, D-37077 Göttingen — [2]Universität Münster, Institut für Materialphysik, D-48149 Münster

Under high electrostatic fields $E$, tip-shaped metal nanowires transform into the corresponding oxide at room temperature if a certain partial pressure $p$ of water is present. A TEM investigation of this reaction was performed on nanowires of tungsten and aluminum as well as silicon.

The oxidation reaction starts at a critical field strength $E_c(p)$ of the order of $10^9$ V/m and proceeds until a quasi stationary state is reached. The kinetics of the reaction is gas supply-limited for pressures below $10^{-3}$ mbar and proceeds with rates corresponding to a diffusion coefficient of the order of $10^{-15}$ m$^2$/s for a vapor pressure in the 10 mbar range, indicating driven diffusion.

Determination of the the electric field distribution inside the oxide using the finite element method and the results of current measurements during the oxidation reaction indicate that the critical step of the oxidation process is a surface reaction at the oxide-vapor interface. A quantitative model describing the observed $E_c(p)$ dependence is given.

MM 23.42 Tue 14:45 Poster B

**Electronic transport properties of nanocomposite materials prepared by electron and ion beam induced deposition** — •Christina Grimm, Dirk Klingenberger, Harald Drings, and Michael Huth — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

A survey is given of the electronic transport properties of tungsten-based nanocomposite materials prepared with electron (EBID) or ion (IBID) beam induced deposition employing $W(CO)_6$ as precursor. The samples are analyzed in the normal state with regard to temperature-dependent electron correlation corrections to the Drude conductivity. A $\sqrt{T}$-dependence of the electrical conductivity was found for the first time in samples prepared by EBID. IBID samples with metal content approaching 50% show superconducting transitions at approx. 5 K. The properties of these samples are analyzed on the basis of the transport theory of Josephson-coupled networks. Finally, recent results on employing these materials for sensor applications are presented.

MM 23.43 Tue 14:45 Poster B

**Lattice dynamics of ferromagnetic shape memory alloys from inelastic neutron scattering** — •Tarik Mehaddene[1], Juergen Neuhaus[2], Winfried Petry[1,2], Klaudia Hradil[2,3], and Philippe Bourges[4] — [1]Physik-Department E13, Technische Universitaet Muenchen, D-85747 Garching, Germany — [2]Forschungsneutronenequelle Heinz Maier-Leibnitz, D-85747 Garching, Germany — [3]Institut fuer Physikalische Chemie, Georg-August-Universitaet, D-37077 Goettingen, Germany — [4]Laboratoire Leon Brillouin (LLB), CEA Saclay, F-91191 Gif sur Yvette Cedex, France

The tendency of shape memory alloys to undergo a martensitic transtion shows up in the anomalous phonon softening of particular phonon modes in their austenitic phase. We report on phonon measurements in both austenitic and martensitic phases of Ni-based alloys. We show that, contrary to NiMnSn, the anomalous softening of the $TA_2$[110] phonons in NiMnGa is strongly enhanced below the Curie temperature. The measurements revealed that low restoring forces against the shearing of the (111) atomic planes along [11-2] develop upon cooling. The vibrational spectra measured in two different martensitic phases of NiMnGa, namely the tetragonal 5M and the orthorhombic 7M structures, revealed fundamental differences. A dispersive low-energy excitation develops from the elastic modulation peaks in the 5M structure and come into interaction with $TA_2$[110] phonon branch in the q-range 0.25-0.3 r.l.u where the latter shows a wiggle in the dispersion. No wiggle is seen in the $TA_2$[110] branch of the 7M structure. It shows a normal sinus-like dispersion curve.

MM 23.44 Tue 14:45 Poster B

**Phase diagrams for the evolution of polydomain and polyvariant states in tetragonal ferromagnetic martensites** — •Aristide T. Onisan[1], Nikolay S. Kiselev[1,2], Ulrich K. Rössler[1], and Alexei N. Bogdanov[1,2] — [1]IFW Dresden — [2]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 magnetic charges arise internally at the twin boundaries. [1] A.N. Bogdanov, A. DeSimone, S. Müller, U.K. Rößler, J. Magn. Magn. Mater. 261 (2003) 204. *Supported by DFG, SPP 1239 project A08.*

MM 23.45 Tue 14:45 Poster B

**Correlated ferroelastic/ferromagnetic domain walls in ultrathin films: observations and physical description** — •Catherine Jenkins[1,2], R Ramesh[1], and Gerhard Jakob[2] — [1]University of California, Berkeley — [2]Johannes 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.

1. Bertram HN, Paul DI, J Appl. Phys., vol.82, no.5, 1997, p. 2439
2. S. J. Murray et al, J. Appl. Phys., vol. 87, No. 9, 2000, p. 5774

MM 23.46 Tue 14:45 Poster B

**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 laser energy absorption 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 an electron-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.

[1] S.I. Anisimov, B.L. Kapeliovich and T.L. Perel'man: Sov. Phys. JETP 39, 375(1974)

MM 23.47 Tue 14:45 Poster B

**Structural Properties of the Metastable State of Phase Change Materials Investigated by Synchrotron Radiation** — •Philipp Merkelbach[1], Julia van Eijk[1], Carolin Braun[2], and Matthias Wuttig[1] — [1]I. Phys. Institut (IA), RWTH Aachen, 52056 Aachen — [2]Institut für Anorg. Chemie, CAU Kiel, 24098 Kiel

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

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 drastical 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 23.48 Tue 14:45 Poster B

**Crystallization kinetics of phase change materials** — •Andreas Kaldenbach, Martin Salinga, Ursula Nellen, Carl Schlockermann, and Jennifer Luckas — I. 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 are not yet understood in all detail. Ironically its most characteristic property, the crystallization kinetics, still has not been determined experimentally beyond a quite limited temperature range around the glass transition temperature and slightly below the melting temperature respectively. The uncertainty about the crystallization behavior in the intermediate temperature regime has so far been coped with by applying existing theoretical equations for a continuous description of nucleation and growth. However, until now these theories have not yet been validated by experimental evidence for the mentioned class of materials. The lack of experimental data is mainly caused by the high crystallization speed of phase change materials being truly demanding in respect to both the heating rates and the detecting system of an experiment. Thus an optical setup is assembled to conduct measurements of the phase change utilizing a pulsed laser. Experimental results are compared with existing theories on crystallization.

MM 23.49 Tue 14:45 Poster B

**Characterization of a FePd single crystal for sensor applications** — •Christoph Bechtold[1], Andreas Gerber[1], Manfred Wuttig[2], Eckhard Quandt[3], Jeff McCord[4], Yiu Wai Lai[4], Jörg Buschbeck[4], Ludwig Schultz[4], Oleg Heczko[4], and Sebastian Fähler[4] — [1]Research Center caesar, Ludwig-Erhard-Allee 2, 53175 Bonn — [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

Magnetic shape memory (MSM) materials have received much attention in actuator applications due to their large strains and short response times. However, their potential as an alternative to conventional magnetostrictors in sensor systems has not been studied so far. A FePd single crystal was characterized by EDX, VSM, DSC and temperature dependent XRD analysis. The magnetic field induced strain under different compressive loads was studied at temperatures ranging from 0 to -40°C and magnetic field induced actuation and twin boundary movement were confirmed and quantified by temperature dependent optical observation in the austenitic and martensitic state. Additional features of the role of magnetic domains on the MSM response will be presented.

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MM 23.50 Tue 14:45 Poster B

**Molecular dynamics simulation study of crystal growth and melting of pure metals** — •Roberto Rozas and Juergen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder 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 Klassen[1], Patrick Wette[1], Dirk Holland-Moritz[1], Dieter M. Herlach[1], Thomas Palberg[2], and Stephan V. Roth[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55128 Mainz, Germany — [3]HASYLAB, DESY, 22603 Hamburg, 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 that 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** — •Nina 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 gravitation 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 takes days to reach its final value in 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.

[1] N.Lorenz, J.Liu, T. Palberg: Phase behaviour of binary mixtures of colloidal charged spheres, Colloids Surf. A (in press 2007)