MM 31: Postersitzung II

Time: Wednesday 17:15–18:45 Location: P5

MM 31.1 Wed 17:15 P5

Structure-optimization of the Ξ-phases in the Al-Pd-Mn system — •Benjamin Frigan[1], Marek Mihalkovič[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

The Ξ-phases – with ξ and ξ' being the simplest ones – are probably the most investigated ternary phases. The experimental structure refinement of ξ' carried out by Boudard et al. dates back more than 10 years. Almost all present studies rely on this structure proposal. Here we present an optimization of the Boudard model using a combination of classical molecular dynamics and density functional theory. We determine an optimal configuration for the Al atoms on the innermost shell of the pseudo-Mackay clusters (PMC). These Al atoms could not be resolved very accurately in experiment. Furthermore, we examine the "glue" atoms, i.e. those not belonging to any PMC. In order to get an estimate for the stability of a phase the ground state energies are calculated relative to other binary and ternary compounds coexisting in the Al-Pd-Mn system. The results are applied to the ξ'_1-phase (ε_{16}) where the projections of the PMC columns form pentagons and nonagons.

MM 31.2 Wed 17:15 P5

Refined model of phason flips in quasicrystals using kinetic Monte Carlo simulations — •Hansjörg Lipp and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

HRTEM observations of decagonal Quasicrystals by Edagawa et al. [1] show that phason flips can be observed directly as spots which vanish or appear erratically. The spots can be interpreted as clusters of atoms, which move coherently. Compared to the time scale of atomic jumps (picoseconds), this process is surprisingly slow, flips occur in periods of seconds or even minutes.

We study this phenomenon using several statistical model systems, e.g. based on a structure model for d-Al-Cu-Co suggested by Zeger et al. [2], where rings of ten atoms can perform flips by collective motion of atoms inside decagonal double layers. Using kinetic Monte Carlo simulations [3], we investigate how flip frequencies depend on the number of decagonal layers and on the variations of the local energy landscape.

[1] K. Edagawa *et al.*, *Phys. Rev. Lett.* **85**, 1674 (2000)
[2] G. Zeger and H.-R. Trebin, *Phys. Rev. B* **54**, R720 (1996)
[3] A. B. Bortz *et al.*, *J. Comput. Phys.* **17**, 10 (1975)

MM 31.3 Wed 17:15 P5

Structural changes of Gd thin films and islands during hydrogen absorption — •Sara Wanjelik, Georg Oeltzschner, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

We report on the effects of hydrogen absorption in Gadolinium Systems by using scanning tunneling microscopy (STM) and spectroscopy (STS).

Offering low amounts of hydrogen (1-2 L) to thin films results in the adsorption on the surface. Adsorbed hydrogen changes the electronic structure of the affected areas due to supression of the surface state of Gd (0001). After the subsequent diffusion of hydrogen into the underlying layer the surface state reappears. This can be observed using STS and STM. This change in the electronic structure causes a voltage dependent corrugation which changes sign at 0.8 V. It was observed that the inversion of the corrugation for islands occurs at higher voltages.

For higher dosage (>50 L) not only the electronic structure is affected but also the topographic structure. As a result we found small circular islands (diameter 6-8 nm) and ramp-like structures exhibiting the height of one atomic step. The topographic change of the surface can be ascribed to hydride formation (GdH_2) in the thin film. This obsevation will be compared to the behavior of islands during hydrogen absorption.

MM 31.4 Wed 17:15 P5

Electrochemical analysis of SiNWs anodes in lithium-ion batteries according to the amount of copper deposition — •Gibaek Lee[1,2], Gaelle Offranc-Piret[3], Fracois Ozanam[3], Stefan L. Schweizer[2], and Ralf B. Wehrspohn[1,2] — [1]Fraunhofer Institute for Mechanics of Materials Halle — [2]Martin-Luther-University Halle-Wittenberg — [3]Ecole Polytechnique, France

It has been known for some time that silicon can incorporate large amounts of Li with a specific capacity of 4200 mAh/g, about a factor of 11 larger than for state of the art graphite anodes. However, silicon and silicon-based negative electrodes exhibit huge volume expansion (ca. 270%) during alloying/de-alloying, resulting in mechanical disintegration of electrode and rapid capacity fading. Addition of inactive but conductive elements into silicon can improve electrical connection of particles and suppress volume change.

In this study, we prepared oriented silicon nanowires (SiNWs) array on n-type silicon substrate by electroless etching in aqueous HF solution containing $AgNO_3$, and then filled in SiNWs, with copper by electrodeposition in aqueous solution. The material characteristics and anodic performance of copper deposited SiNWs anodes have been examined.

MM 31.5 Wed 17:15 P5

Band engineering for thermoelectric materials — •Mingxing Chen and Raimund Podloucky — Faculty of Chemistry, Univ. Vienna

Engineering of the electronic band structure of Ge-based skutterudites and clathrates is of importance for optimizing their thermoelectric properties in terms of Seebeck coefficients. Alloys of $FM_4Sb_xGe_{12-x}$ skutterudites and $Ba_8M_xGe_{46-x}$ clathrates (F: filler atom, M: metal) are investigated by means of density functional theory calculations from which the transport properties are derived by Boltzmann transport theory within the constant relaxation time approach[1]. For a large Seebeck coefficient it is important to place the Fermi energy close to a gap. Therefore, we analyse the nature of gap formation for these two classes of materials and derive a simple counting rule for chemical optimization of the thermoelectric properties [2]. Following this rule, our data on skutterudites reveal that partially replacing Ge by Sb leads to the desired placement of the Fermi energy. For clathrates, also the electric resistivities are analyzed which reveal characteristic temperature dependent features in agreement with experiment[2].

[1] G. K. Madsen and D. J. Singh, Comput. Mater. Sci. 175, 67 (2006). [2] I. Zeiringer, Mingxing Chen et al., submitted.

MM 31.6 Wed 17:15 P5

Epitaxy, lift-off and surface treatment of Ni-Mn-Ga based magnetic shape memory alloy films — •Marcus Müller and S. G. Mayr — Leibniz-Institut für Oberflächenmodifizierung, Translationszentrum für regenerative Medizin und Fakultät für Physik und Geowissenschaften der Universität Leipzig, 04318 Leipzig

During the past years much progress has been achieved in the field of magnetic shape memory alloys. The Ni-Mn-Ga alloy is presumably the most prominent representative, which can yield strains as high as 10% in highly tailored single crystals. Freestanding miniaturized single crystalline films on the other hand are much less explored and face several challenges, particularly including single crystalline growth and film lift-off. Using magnetron sputtering from Ni-Mn-Ga compound target we fabricate single-crystalline-like epitaxial Ni-Mn-Ga films on a heated MgO (100) substrate, which transform to the martensite phase upon cooling down to room temperature [1]. A recently-developed etching technique [2] for direct removal of the MgO substrate is subsequently employed for lifting these films off the substrate, which is currently being optimized further. As a main advantage the present approach does not require buffer layers, which would possibly prove harmful at the elevated temperatures employed for epitaxy. With the aim of enhancing biocompatibility, coating concepts are furthermore explored.

[1] G. Mahnke, M. Seibt, S.G. Mayr, Phys. Rev. B 78, 012101 (2008)
[2] T. Edler, S.G. Mayr, Adv. Mat. (in press, 2010)
This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909.

MM 31.7 Wed 17:15 P5

Proton conductivity of imidazole molecules encapsulated in

imogolite nanotubes. — •Barbara Supronowicz, Agnieszka Kuc, and Thomas Heine — SES, Jacobs University Bremen, Bremen, Germany

Proton conduction in solids has gained a lot of attention because of promising variety of applications, such as proton exchange membranes (PEMs) and fuel cells.[1a] The choice of PEM has an influence on the efficiency of fuel cell. Due to stability and electronic properties[2] imogolite has been chosen as a host structure for proton carriers. The presence of water molecules has a significant influence on the proton conductivity[3]. To avoid the dependence of proton conductivity on the temperature, different proton carrier * imidazole * was introduced into the structure instead of water molecules.[1]

All the structures were investigated using SCC- DFTB method.[4]

[1] a) Kreuer, K.D. Chem. Mater. 1996, 8, 610-641. b) Goward, G.R., et al. J. Phys. Chem.B.,2002, 106, 9322-9334.

[2] Guimaraes, L.; Enyashin, A.N.; Frenzel, J., et al. ACS NANO, 2007,1, 362-368.

[3] Cukierman, S.; Biochimica et biophysica acta- bioenergetics, 2006, 1757, 876-885.

[4] Elstner, M; Porezag, D. et al. Phys. Rev. B.,1998, 58, 7260-7268.

MM 31.8 Wed 17:15 P5

Evaluation of perovskite oxides as oxygen evolving catalyst for photocatalytic water splitting — •Daniel Mierwaldt[1], Jörg Hoffmann[1], Bruno Jasper[1], Christian Jooss[1], Stephanie Raabe[1], Sven Schnittger[1], and Simone Techert[2] — [1]Institut für Materialphysik, Universität Göttingen — [2]MPI für biophysikalische Chemie, Göttingen

In search for suitable water splitting catalysts, several oxide materials have already been successfully investigated. However, most of them have band gaps in the UV-region limiting the efficiency in light harvesting. Perovskite manganites represent a promising material class, in which strong electron-lattice coupling results in a broad polaronic absorption band from visible light to near-IR. In addition, multilevel excitation into long-living polaronic states may contribute to high chemical potentials of electron-hole pairs, exceeding the band gap of the respective material.

In this contribution the strongly correlated $CaMnO_3$ has been investigated, which reveales a rather large exchange current density of about 1,9 mA/cm^2. Bulk samples as well as epitaxial grown thin films on Nb-doped $SrTiO_3$ substrate were investigated by means of cyclic voltammetry. The samples were used as working anode in a photocatalytic apparatus with Pt-counter cathode in Na_2SO_4-electrolyte.

A complementary approach to water splitting is the use of nano composites forming two dimensional patterns of pn-junctions. First results on the photocatalytic activity of Nb-doped $SrTiO_3$ (n-type) mixed with off-stoichiometric $CoFe_2O_4$ (p-type) are presented.

MM 31.9 Wed 17:15 P5

Niobium doped SrTiO3 and p-type CoFe2O4 nanocomposite films for photoelectric applications — •Bruno Jasper, Daniel Mierwaldt, Andreas Blumenstein, Sven Schnittger, Jörg Hoffmann, and Christian Jooss — Institute of Material Physics, University of Göttingen, Germany

Patterned arrays of pn-junctions are interesting model systems for the study of photocatalytic and photovoltaic applications. In this field, self-organizing systems show promising results with respect to simple preparation and increasing efficiency. As an example of self-organized oxide structures we present a study of nanocomposites composed of strontium titanate (SrTiO3) and cobalt ferrite (CoFe2O4) prepared by reactive ion beam sputtering. Doped SrTiO3 is a photoactive material allowing water splitting. Properly doped CoFe2O4 is a good conductor which serves well as a catalyst in hydrogen production. Voltage-cyclometric measurements reveal photo-catalytic activity of single phase Nb:SrTiO3 as well as the SrTiO3-CoFe2O4 nanocomposite films. Furthermore, first results on the fabrication of n-type niobium doped strontium titanate (Nb:SrTiO3) and off stoichiometric p-doped cobalt ferrite (p:CoFe2O4) by self-organized decomposition are presented. The structural and chemical properties of the samples are examined by scanning electron microscopy, X-ray diffraction, transmission electron microscopy and energy dispersive X-ray spectroscopy.

MM 31.10 Wed 17:15 P5

Material Test Facilities for Solar Absorber of Solar Tower Power Plants — Bernhard Hoffschmidt, Konstantin Konstantin Geimer, Oliver Kaufhold, and •Markus Sauerborn — Solar-Institut Jülich (SIJ), FH Aachen, Heinrich-Mußmann-Str. 5, D-52428 Jülich

Since 2009 the first and only German solar tower power plant the large scale test facility Solar Tower Juelich is in operation. The SIJ has initiated the construction phase and is now with the German Aerospace Center/DLR exclusive involved in the accompanying research. The central receiver plant features as central innovation an open volumetric receiver, consisting of porous ceramic elements that simultaneously absorb the concentrated sunlight and transfer the heat to ambient air passing through the pores so that an average temperature of 680°C is reached. The subsequent steam cycle generates up to 1.5MWe. To analyze the capability of new absorber specimen under realistic conditions or optimize the structures several special labor test facilities had been developed at the SIJ. An interesting one is using a powerful near-infrared radiator to simulate concentrated solar light. It offers a beam power of up to 300W/m* for test samples with a surface of about 14x14cm and the absorber surface can reach more than 1000°C. To suck ambient air through the open absorber - like on the tower - it is mounted on a special compressor system. An easy and quick change of the absorber specimen makes it possible to test new absorber structures fast and reproducible under various radiation conditions. An overview about the test facility and some results of the last years will be given.

MM 31.11 Wed 17:15 P5

SIMS study on the surface elemental distribution in AISI type 304 steel — •Chika Izawa[1], Stefan Wagner[1], Vladimir Burlaka[1], Mauro Martin[2], Sebastian Weber[2], Anais Bourgeon[3], Richard Pargeter[3], Thorsten Michler[4], and Astrid Pundt[1] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Gemeinsame Forschergruppe, Helmholtz-Zentrum Berlin / Ruhr-Universität Bochum, Universitätsstr. 150 - IA 2/44, D-44801 Bochum — [3]TWI Ltd, Granta Park, Great Abington, Cambridge CB21 6AL, United Kingdom — [4]Adam Opel GmbH, IPC R2-50, GM Alternative Propulsion Center Europe 65423 Ruesselsheim

Hydrogen embrittlement of low-Ni austenitic stainless steels is suggested to occur due to strain-induced surface alpha -martensite, since the hydrogen diffusivity in bcc phases is expected to be much higher than in the austenitic phase. But, also the local surface chemistry might be responsible for the steel susceptibility. The surface chemistry on two different surface conditions of AISI 304 was investigated by Secondary Ion Mass Spectrometry: a. directly after the machining process and b. after solution annealing process. For both AISI 304 surfaces a layered stacking of Fe- and Cr-oxide was found. The oxide layer thickness was about 5 nm for sample a., and about 10 nm for sample b. The chemical mapping on sample a. shows relatively homogeneous elemental distributions due to the fine microstructure of martensite. For sample b, Fe, Ni, SiO2, FeO and NiO are segregated at the grain boundaries. In contrast, Cr and CrO are distributed in grains.

MM 31.12 Wed 17:15 P5

Gezielte Strukturmodifizierung der MOFs zur Optimierung von Sorptionseigenschaften — •Olga Khvostikova[1,2], Lars Giebeler[1], Bassem Assfour[3], Gotthard Seifert[3], Helmut Hermann[1] und Helmut Ehrenberg[1] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 27 01 16, D-01171 Dresden, Germany — [2]Institut für Werkstoffwissenschaft, TU Dresden, Helmholtzstr. 7, D-01069 Dresden, Germany — [3]Institut für Physikalische Chemie, TU Dresden, Bergstr. 66b, D-01062 Dresden, Germany

MOFs sind eine relativ neue Verbindungsklasse in der Festkörperchemie, wobei die Abkürzung MOF für Metal-Organic Framework, metallorganische Gerüststruktur, steht.

Wasserstoffspeicherung in diesen hochporösen Materialien wird als eine vielversprechende Strategie für die Entwicklung der on -board Technologie bei Kraftfahrzeugen betrachtet.

Die Herstellung von Materialien mit kleinen Poren, das Dotieren mit hydrogenophilen Metallen, ein anderes Konnektorkation oder die Variation von Brückenliganden sind mögliche Wege zur Optimierung der Materialien und der Erzeugung von effektiven Wasserstoffspeichern.

Im Rahmen der Forschungsarbeit werden MOF - Materialien zur Bestimmung der Einflüsse von unterschiedlichen Strukturparametern und Präparationsverfahren auf die Wasserstoffspeicherkapazität gezielt hergestellt und auf ihre Wasserstoffspeichereigenschaften untersucht.

MM 31.13 Wed 17:15 P5

Hydrothermal synthesis and physical properties of LiXPO4

(X = Mn, Fe, Co, Ni or mixtures) — •Carsten Jähne[1,2], Christine Täschner[2], Bernd Büchner[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, 69120 Heidelberg — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden

Due to their high open circuit voltages (OCV), materials with phosphor olivine structure are of great interest for application as positive-electrodes in secondary batteries. However, the low electrical conductivity of olivine materials results in a low power capability which demands downscaling of the crystallites in order to enhance surface to volume ratio and/or appropriate post-treatment techniques. Here we report on low temperature conventional and microwave-assisted hydrothermal synthesis of LiXPO4 (X = Mn, Fe, Co, Ni or mixtures of these). In particular, we present electron microscopy, x-ray diffraction and magnetization data on the resulting material which allow to determine the phase, the morphology and the valence of the transition metal ions.

MM 31.14 Wed 17:15 P5

Deuterium trapping in graphite and carbon films growing under irradiation by deuterium plasma — •Vladimir Burlaka[1,2], Yuriy Gasparyan[2], Aleksandr Pisarev[2], Aleksandr Rusinov[2], Stepan Krat[2], and K. Sugiyama[3] — [1]University of Goettingen, Germany — [2]National Research Nuclear University "MEPhI", Moscow, Russia — [3]Max-Planck-Institut für Plasmaphysik, Garching, Germany

Carbon is planned to be used in the divertor of ITER until the tritium phase. Its further use is under discussion for possible high tritium inventory. In the case of graphite or other carbon-based materials, essentially four mechanisms have been identified for the uptake and retention of hydrogen: buildup of a saturated surface layer, chemisorption on inner porosity surface, intergranular diffusion and trapping, and co-deposition of hydrogen with carbon on plasma-exposed surfaces. This work was motivated by the investigation of hydrogen trapping in graphite and co-depositing carbon films growing by the plasma irradiation. A new laboratory plasma device for investigation of plasma surface interaction was constructed. Ion pickup research, surface modification, re-deposition of the sputtered material and combined carbon and hydrogen deposition from the plasma, were performed. Used analysis techniques: thermal desorption spectroscopy (TDS), SEM, AFM and Nuclear reaction analyses (NRA).

MM 31.15 Wed 17:15 P5

SIMS study on the surface elemental distribution in AISI type 304 steel — •Chika Izawa[1], Stefan Wagner[1], Vladimir Burlaka[1], Mauro Martin[2], Sebastian Weber[2], Anais Bourgeon[3], Richard Pargeter[3], Thorsten Michler[4], and Astrid Pundt[1] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Gemeinsame Forschergruppe, Helmholtz-Zentrum Berlin / Ruhr-Universität Bochum, Universitätsstr. 150 - IA 2/44, D-44801 Bochum — [3]TWI Ltd, Granta Park, Great Abington, Cambridge CB21 6AL, United Kingdom — [4]Adam Opel GmbH, IPC R2-50, GM Alternative Propulsion Center Europe 65423 Ruesselsheim

Hydrogen embrittlement of 8 wt-% Ni, 18 wt-% Cr austenitic stainless steels is suggested to occur due to strain-induced surface $\alpha-$martensite, since the hydrogen diffusivity in bcc phases is expected to be much higher than in the austenitic phase. But, also the local surface chemistry might be responsible for the steel susceptibility. The surface chemistry on two different surface conditions of AISI 304 was investigated by Secondary Ion Mass Spectrometry(SIMS): a. directly after the machining process and b. after solution annealing process. The chemical mapping on sample a. shows relatively homogeneous elemental distributions due to the fine microstructure of martensite. For sample b, larger grains are observed. At the grain boundaries, Fe, Ni, SiO_2, FeO and NiO are segregated. In contrast, Cr and CrO are distributed in grains. Financial support from the Bundesministerium für Wirtschaft und Technologie (BMWi), 0327802C is gratefully acknowledged.

MM 31.16 Wed 17:15 P5

Intercalation Mechanism and Aging Effects in LiFePO4 as Cathode Material for Li-Ion-Cells — •Birte Riechers, Sebastian Mathes, Carsten Nowak, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen, Germany

Since Lithium Iron Phosphate was recently established as a cathode material for high-current Li-Ion cells, intercalation mechanisms and aging effects in this material come to the forefront of scientific investigations. An enhanced understanding of time- and cycling-mode dependent changes of Li-intercalation processes of LiFePO4 contributes to these efforts. Using commercial, self-prepared, and thin-film model Li-ion cells, microstructural changes and aging effects are investigated using (in-situ) SEM, XRD.

The progress of degradation depending on electrolyte, method of cell preparation, and cycling conditions is studied. The homogeneous intercalation structure of pristine cells changes to a spatially heterogeneous structure due to different intercalation kinetics and phase distributions. This occurs even within single cathode material particles. Thin-film model cell cathode intercalation processes are being compared to the behaviour of cathodes consisting of particles.

MM 31.17 Wed 17:15 P5

Investigation of the heterogeneous nucleation in the peritectic AlNi alloys — •Julia Kundin[1], Hai-Lin Chen[2], Heike Emmerich[1], and Rainer Schmid-Fetzer[2] — [1]Material and Process Simulation (MPS), University Bayreuth, Germany, Nürnberger str.38(4) 95448 Bayreuth — [2]TU Clausthal, Inst. Metallurgie, Robert-Koch-Str. 42 38678 Clausthal-Zellerfeld Germany

A quantitative multi-phase field model is used for the simulation of the solidification and for stages of peritectic transformation in the binary Al-Ni alloy. The experimental DSC curves were used for the calibration of the model and the evaluation of the kinetic parameters and the nucleation rate. For the simulation of the heat flow the temperature correction method have been employed. The model can be employed to obtain new relations between processing parameters and resulting kinetics and dynamics of the phase-transformation processes. The model and the method of the calibration could be applicable to any alloy systems with the known thermodynamic data.

MM 31.18 Wed 17:15 P5

Exploring the interface structure of TaN/Gd_2O_5/HfO_2 gate stacks — •Catharina G. Wille, Dongkyu Cha, J. Alfonso Caraveo, Husam N. Alshareef, and Tala'at Al-Kassab — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

The recent introduction of high dielectric constant (high-k) oxides such as HfO_2 as replacement materials for the SiO_2 gate dielectric has accelerated research activity in high-k materials for transistor-based devices.

In this study, a Gd_2O_5/HfO_2 stacked gate dielectric was used to fabricate TaN/ Gd_2O_5/HfO_2 /SiO_2/Si thin films and MOS capacitors. The effects of annealing condition on the structure and morphological properties of the proposed films were investigated via transmission electron microscopy (TEM). As shown in earlier works, DFT calculations in conjunction with the electrical and physical characterization of the gate stacks demonstrated the importance of controlling the distribution of both oxygen and nitrogen atoms directly at the TiN/HfO_2 interface.

With the addition of the Gd_2O_5 -layer, the oxygen concentration depth profile was derived both by means of electron energy loss spectroscopy (EELS) and atom probe tomography (APT). Structural investigation by means of high resolution transmission electron microscopy (HR-TEM) concluded the detailed study of the metal/dielectric interface.

MM 31.19 Wed 17:15 P5

Simulation of structural transitions in NiTi systems — •Daniel Mutter and Peter Nielaba — University of Konstanz, 78457 Konstanz, Germany

In this work, we performed atomistic molecular dynamics simulations of the structural phase transition in NiTi alloys between B19' at low and B2 at high temperatures [1]. To this end, a semi-empirical potential from the literature was adopted [2] and modified, which is based on the tight-binding model in second moment approximation. We present an analysis of crystallography and energetics of the emerging structures during a heating-cooling cycle, which is applied to systems with 2048 atoms under periodic boundary conditions. The experimentally known strong dependence of transition temperatures (TTs) on alloy composition is confirmed and related to an increasing lattice instability, arising when the perfect ordered composition with 50% Ni and 50% Ti is changed slightly. By applying free boundary conditions, spherical NiTi nanoparticles with diameters between 3 and 17 nanometers were simulated, where a size dependence of the TTs was observed. In

order to explain this behavior, an order parameter for distinguishing locally between B19' and B2 was constructed, with which a visualization of the phase transition was possible, showing that the start of the structural transformation is mainly triggered by the surface of the nanoparticle.

[1] D. Mutter and P. Nielaba, Phys. Rev. B 82, 224201 (2010).
[2] W.S. Lai, B.X. Liu, J. Phys. Cond. Mat. 12, L53-L60 (2000).

MM 31.20 Wed 17:15 P5

Interaction of ultrashort XUV pulses with bulk magnesium — •Naira Grigoryan, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

A recently published experimental work (Nagler et al.) shows that the excitation of a material with very intense femtosecond XUV pulses first leads to an exotic state characterized by a very high density of core holes (about 1 core hole per atom) and relatively warm electrons. The next step is the formation of warm dense matter. In this work we perform all-electron ab-initio calculations to determine the main pathways from solid to warm dense magnesium. We simulate the XUV excitation by constructing a state with hot electrons and core holes. By analyzing particular optical and acoustic phonon modes at high symmetry points of the Brillouin zone in the highly excited electronic state as a function of the electronic temperature and the number of core holes we obtain an indication of the atomic pathways involved in the first stages of the formation of warm dense matter.

MM 31.21 Wed 17:15 P5

X-ray Raman Scattering Studies of Si-based Compounds Under Extreme Conditions — •Christoph Sahle[1], Christian Sternemann[1], John Tse[2], Max Wilke[3], Christian Schmidt[3], Alexander Nyrow[1], Julien Dubrail[3], Valentina Giordano[4], Laura Simonelli[4], Serge Desgreniers[5], and Metin Tolan[1] — [1]Fakultät Physik/DELTA Technische Universität Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Germany. — [2]Department of Physics, University of Saskatchewan, Saskatoon S7N0W0, Canada. — [3]Geoforschungszentrum Potsdam, Telegraphenberg, 14773 Potsdam, Germany. — [4]ESRF, Rue Jules Horowitz, 38043 Grenoble Cedex, France. — [5]Laboratoire de physique des solides denses, University of Ottawa, Ottawa K1N6N5, Canada.

The *in situ* study of low Z elements' absorption edges under extreme conditions is only feasible using hard x-rays. Here, non-resonant x-ray Raman scattering as an energy loss technique enables one to choose the energy of the primary x-ray beam freely and thus gives access to shallow absorption edges of samples in highly absorbing sample environments, e.g. diamond anvil cells, which do not permit electrons and soft x-rays as probe. Here, we present two studies of Si-based compounds under extreme conditions: a high pressure study of the peculiar phase transitions in silicon clathrate Ba_8Si_{46} via measurements of the Ba N_{45} and Si L_{23} edges. In addition, we present the first *in situ* high pressure – high temperature study at the Si L_{23} and Na L_{23} edge on hydrous $Na_2Si_3O_7$ melt, which may serve as a model for geologically relevant hydrous silicate melts in the deep earth.

MM 31.22 Wed 17:15 P5

Towards the study of electric field gradients in M_2AlC (M = Ti, Nb, V, Cr) MAX phases — •Daniel Jürgens[1], Christoph Brüsewitz[1], Michael Uhrmacher[1], Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]Georg-August-Universität Göttingen, II. Phys. Inst., Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

Layered ternary carbides like Ti_2AlC and Nb_2AlC have attracted great attention in recent time. These materials belong to the MAX phase family whose compounds show an unique combination of both metal- and ceramic-like properties. Some features are their excellent thermal and electrical conductivity even at high temperatures, their low density and high oxidation resistance as well as their easy machinability. The purpose of this work is to describe and understand their physical behavior on atomic scale since many investigations came to the conclusion that the observed characteristics on the mm or even μm scale have their origin in the microstructure. To do so the technique of perturbed angular correlation (PAC) was used beside XRD to gain detailed information about the atomic environment. Radioactive ^{111}In ions, decaying by a γ-γ cascade, were implanted into the samples, sensing as *spies* their local surrounding via hyperfine interactions. This method was applied to Ti_2AlC, Nb_2AlC, V_2AlC and Cr_2AlC. In each material an axially symmetric EFG was found with a characteristic quadrupole coupling constant ν_Q variing between 180 MHz and 260 MHz, which decreases linearly with increasing measurement temperature. This work is supported by the DFG under contract HO 1125/19-1.

MM 31.23 Wed 17:15 P5

Phase-field study of needle crystal fragmentation — •Marius Kist[1], Abhik Choudhury[1], and Britta Nestler[1,2] — [1]Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Moltkestr.30, 76133 Karlsruhe, Germany — [2]Institute of Reliability of Components and Systems(IZBS), Karlsruher Institut für Technologie, Haid-und-Neu-Str.7, 76131 Karlsruhe, Germany

We investigate the melting process of a single solid phase in contact with its liquid for the case of a binary alloy at near to equilibrium conditions by two and three dimensional simulations based on a phase-field method. In particular, we study the effect of surface energy anisotropy on the melting behavior. In 2D, for the case of isotropic surface energies, the solid phase melts continuously keeping its shape intact. For the case of anisotropic surface energy giving rise to elliptical needle crystals, we observe a discontinuous melting behavior where, beyond a critical aspect ratio (major axis/minor axis), the needle splits into two fragments while melting. We investigate this phenomenon, and suggest a mechanism for its occurrence. In 3D, the classical Rayleigh-Plateau-Instability is known to cause a break up of a cylindrical surface into a row of droplets through surface energy minimization. This instability is an additional contribution to the splitting behavior of needle crystals. We study the interplay of the mechanisms of needle breaking in 2D and analyze the effect of Rayleigh Instability in the presence of bulk diffusion in 3D. From the phase-field simulations, we derive the time exponent for the kinetics of the needle crystal fragmentation.

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Ti-based dendrite - nano/ultrafine eutectic composites: microstructure control via semi-solid processing — •Olga Shuleshova[1], Norbert Mattern[1], Wolfgang Löser[2], and Jürgen Eckert[1,3] — [1]Institute for Complex Materials, IFW Dresden, Germany — [2]Institute for Solid State Research, IFW Dresden, Germany — [3]Institute of Materials Science, TU Dresden, Germany

Recently, considerable advances are achieved in ductilization of the inherently brittle high-strength materials, such as metallic glasses and nano/ultrafine eutectics, through incorporation of soft dendritic phase, which primarily solidifies from the melt and is subsequently embraced in a strong matrix. An enhanced mechanical properties results from cooperative interplay of the inhomogeneous microstructure with the different deformation mechanisms of the respective phases, and thus are inherently related to the volume fraction, spatial sizes, morphology and overall distribution of the ductile crystalline phase reinforcement. Present work explores the possibility to control these parameters via isothermal holding between the liquidus and solidus temperature followed by rapid cooling of the semi-solid mixture. Previously applied only for the metallic glasses composites this approach is adopted here for the Ti-Fe-(Nb) system, known to form nano/ultrafine eutectic at moderate cooling rates. Moreover, relative simplicity of this system allows to study the peculiarities of the microstructures accessible via semi-solid processing in tight connection with the high-temperature phase equilibria given by thermodynamic description of the corresponding systems.

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Differences of the evaporation field in dependence of the crystallographic direction in Al and W by means of Atom probe tomography — •Torben Boll[1,2] and Talaat Al-Kassab[1,2] — [1]Division of Physical Sciences and Engineering King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In field ion microscope (FIM) images the dependence of the brightness of the crystallographic direction is easily observed. This difference in brightness can be related to the evaporation fields at different poles. However this approach allows only a rough qualitative estimation. In this paper an approach will be presented, which utilizes the newly available Wide Angle Atom Probe Tomography (WA-APT) to identify quantitative relations.

The method will be discussed for pure Al- and W-samples. The results are relevant for the development of reconstruction algorithms in WA-APT. Current instruments can analyze a projection angle of about 70° compared to 20°, which was state of the art 10 years ago. Thus

the assumption of hemispherical, symmetrical tips for the reconstruction is not valid anymore. Evaporation fields can be used to identify a complex tip shape and lead to more accurate reconstructions.

MM 31.26 Wed 17:15 P5

Micro-fabricated arrays of SU-8 capillaries with electroplated front electrodes — •Katharina Huhn, Markus Piechotka, Torsten Henning, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392 Giessen

We manufactured thin capillaries out of the negative resist SU-8 with multiple step photolithography. To avoid the formation of stress cracking, a special photomask pattern was designed. The inner diameter of the capillaries varied from 10 to 20 microns whilst the height was in the range of 40 to 100 microns. Afterwards a metal grid structure was deposited onto the top surface of the capillaries using evaporation and lift-off techniques as well as electro-plating.

The aim of this work is to study the feasibility of this method to produce an ionic liquid emitter. SU-8 with its high aspect ratio and easy handling suits the required conditions well. Additionally, SU-8 provides an electric isolating behaviour as needed.

To investigate the shape accuracy and possible defects we used optical, atomic force (AFM) as well as scanning electron microscopy (SEM).

MM 31.27 Wed 17:15 P5

Study of the silver ion release from antimicrobial nanosilver (nAg)/PTFE two dimensional (2D) model — •Nisreen Alissawi[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Dieter Garbe-Schönberg[2], and Franz Faupel[1] — [1]Institute for Materials Science-Multicomponents Materials, Christian-Albrechts-University, Kaiserstr.2, 24143, kiel — [2]Dept. of Geology/ ICPMS Lab, CAU Kiel, Ludewig- Meyn-Strasse 10, 24118 Kiel

Despite the great interest in silver based antimicrobial nanocomposites, it is still not clear how the composite morphology (nanoparticle size, concentration, and distribution) affect the mechanism and kinetics of the interfacial ion transfer reactions of the Ag nanoparticles due to the fact that metal nanoparticles embedded in a polymeric matrix are not directly accessible concerning their interfacial structure and reactivity. This problem will be approached in our present work by the usage of well defined model systems consisting of 2D nanoparticle arrays which are either directly accessible or covered by polymer barrier. The Ag nanoparticles and the PTFE polymer layers were synthesized by physical vapor deposition (PVD) techniques. The samples' morphology, optical properties and composition were examined by Transmission Electron microscopy (TEM), UV-Visible Spectroscopy (UV-Vis) and X-Ray Photoelectron Spectroscopy (XPS), respectively, and the time-dependent release of silver ions after inserting in water was measured using Inductively coupled plasma mass spectrometry (ICP-MS). Time dependence of silver ions release on the particle size and barrier properties are discussed.

MM 31.28 Wed 17:15 P5

Shear-stress induced grain boundary motion in nanocrystalline $Pd_{90}Au_{10}$ — •Manuel Grewer[1], Aaron Weis[2], and Rainer Birringer[1] — [1]Universität des Saarlandes FR 7.2 Experimentalphysik, Saarbrücken, Deutschland — [2]Karlsruher Institut für Technologie - Institut für Nanotechnologie, Eggenstein-Leopoldshafen, Deutschland

The role of shear stress as a driving force for grain boundary migration is a topic which is currently attracting much attention [1,2]. The miniaturized shear compression specimen [3] is a versatile tool to impose large shear deformation during mechanical testing. This shear deformation is strongly localized in the gauge section of the test specimen. Thus it provides an appropriate testing geometry to study grain boundary migration in nanocrystalline materials under dominant shear stress. We investigate the evolution of the grain size distribution function, which has been derived from TEM dark field images, before and after plastic shear deformation of nanocrystalline $Pd_{90}Au_{10}$ with an initial grain size of 10 nm. We find clear evidence for shear deformation driven grain boundary migration at room temperature and >15% plastic strain.

[1] J.W. Cahn et al., Acta mater. 54 (2006), 4953-4975, [2] T.J. Rupert et al., Science 326 (2009), 1686-1690, [3] M. Ames et al., Mater. Sci. Eng. A 528 (2010), 526-532

MM 31.29 Wed 17:15 P5

Thermal stability of indium nanoparticles embedded in an aluminum matrix — •Mostafa Mohamed, Martin Peterlechner, Joachim Bokloh, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-University Münster, 48149 Münster,Germany

The thermodynamics of nanoscaled systems have drawn considerable scientific attention due to the strong influence of the particle size and shape. In the present work, nanoparticles of indium embedded in an aluminum matrix were processed by rapid quenching using the melt-spinning technique. The as-processed samples were analyzed using conventional and analytical transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). TEM data revealed isolated and mainly spherical nanoparticles of indium with a size in the range of 20 to 300 nm. Indium particles in aluminum grains are equiaxed, whereas particles at aluminum grain boundaries show elongation. Analytical TEM showed neither a notable concentration of indium in the aluminum matrix nor a concentration gradient at the interfaces of the particles. By DSC experiments using a wide range of different constant heating and cooling rates, broad melting and crystallization peaks were observed. A slight reduction of the melting temperature of the embedded particles in comparison to the bulk indium is detected, whereas the crystallization temperature shifts to remarkable low temperatures. Upon thermal cycling, the melting as well as the crystallization temperatures of the nanoparticles reduces and the peak shape changes clearly.

MM 31.30 Wed 17:15 P5

Modelling of pine-tree nanowires — •Rainer Schulz[1,2] and Robert Spatschek[1] — [1]Max-Planck Institut für Eisenforschung GmbH, Düsseldorf — [2]ICAMS, Ruhr-Universität Bochum

Nanowires are thin wires (e.g. metal) which are severely restricted in 2 dimensions of space and show a one-dimensional quantization of conductivity. They have a length to diameter ratio of about 1000 and a thickness of some nanometers. Often, they grow defect-free in a catalytic reaction from a substrate, but recently interesting patterns have been observed in situations, where the wires grow in a controlled way with a screw dislocation inside the trunk. As had been predicted earlier, this leads to the so called Eshelby twist of the wire, which stabilizes the dislocation in the center of the wire, and experimental findings suggest that this torsion favors the emergence of sidebranches. In this study we use finite element methods and Ginzburg-Landau models to investigate the dislocation motion and morphology evolution of the nanowire numerically and compare the results to theoretical predictions.

MM 31.31 Wed 17:15 P5

Synthesis and characterization of functional metal oxide nanowires — •babak nasr, subho dasgupta, di wang, robert kruk, and horst hahn — Karlsruher Institut für Technologie, Institut für Nanotechnologie, D-76344 Eggenstein-Leopoldshafen,Germany

Semiconducting metal oxide nanowires (NWs) like SnO2, In2O3, ZnO have found a wide range of applications in electronic devices, such as varistors, gas sensors and lithium ion batteries. Doping with appropriate elements, such as indium (In), antimony (Sb) and tantalum (Ta) can change their optical and electrical properties. In this work undoped and doped SnO2 NWs were synthesized on (100) Si substrates by a catalyst-mediated vapor-liquid solid (VLS) process. Tin oxide*indium oxide NWs were successfully obtained at a constant gas flow rate (O2 1% and Ar, 99%, 100 sccm), 800*900°C temperature window and a growth time of 10 min. The impact of catalyst size on NW*s thickness was studied and it was found that smaller catalyst particles result in thinner NWs. The thickness of NWs was evaluated through scanning electron microscopy (SEM). The crystallographic structure, single crystallinity and growth direction were studied using X-ray diffractometry (XRD) and high-resolution*transmission microscopy (HRTEM) respectively. Well-defined lattice fringes suggested the growth direction along [101]. Compositional analyses via x-ray photoemission spectroscopy (XPS) and Rutherford backscattering spectroscopy (RBS) showed the presence of Sn and Sb as dopant. The NWs were aligned on a patterned substrate for further electrical characterization.

MM 31.32 Wed 17:15 P5

Magnetoconductivity of ferromagnetic thin film samples probed by scanning microwave microscopy — •Stephan Streit[1], Ferry Kienberger[2], Hans-Peter Huber[2], Matthias Fenner[3], Heidemarie Schmidt[1], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01314 Dresden — [2]Agilent Technologies Austria GmbH, Aubrunner-

weg 11, A-4040 Linz, Austria — [3]Agilent Technologies Inc., 61476 Kronberg, Germany

Due to the miniaturisation of electrical devices, measurement techniques need to keep pace to achieve an appropriate spatial resolution. Scanning Microwave Microscopy (SMM) [1] offers the possibility to combine impedance measurements with the advantages of atomic force microscopy. In our work we use a SMM in contact mode to investigate the magnetoconductivity of ferromagnetic thin films. The samples have been prepared by electron beam deposition of iron, cobalt, or nickel films and a Cr protection layer on ZnO substrates. Our quantitative simulation is based on the dependence of the microwave reflection coefficient S11 on conductivity and permeability of ferromagnetic materials [1]. The influence of multiple microwave reflections [2] on the S11 coefficient has been tested for 10 and 20 nm thick ferromagnetic films.

[1] H. Melikyan et al., Ultramicroscopy 108 (2008) 1030-1033 [2] D.M. Pozar, Microwave Engineering, Wiley&Sons, 2005

MM 31.33 Wed 17:15 P5

Influence of the preparation technique on the temperature induced phase separation and nanocrystal formation in $Si_xGe_yO_z$ — •Alexander Nyrow[1], Alexander Schwamberger[1], Christoph J. Sahle[1], Christian Sternemann[1], Achim Hohl[2], Patrick Degen[3], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Experimentelle Physik Ia, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]Institute for Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany — [3]Physikalische Chemie II, Technische Universität Dortmund, Otto-Hahn-Str. 6, 44227 Dortmund, Germany

Since the discovery of visible luminescence from nanocrystallized Si in the early 90s, the study of group IV semiconductor/oxygen systems has received great attention. Due to their unique electronic properties Ge and Si nanocrystals (NCs) are promising candidates for, e.g., light emitting diodes or fast and stable non-volatile flash memory devices. Despite the intensive research regarding the electrical and optical properties of nanoparticles embedded in oxide matrices, spectroscopic studies of its formation process are rare. The NC formation is induced by thermal annealing of the amorphous precursors. It is already known that the composition and the local structure of $Si_xGe_yO_z$ and thus the phase separation essentially depend on the preparation process. To investigate the influence of the preparation technique on the NC formation, samples with various Si/Ge ratios were prepared by evaporation of GeO_2 and Si and by thermal processing of polymers derived from phenyl trichlorogermane and phenyl trichlorosilane, respectively.

MM 31.34 Wed 17:15 P5

Influence of magnetic gradient fields on the electrodeposition of metallic layers — •Kristina Tschulik[1,2], Franziska Karnbach[1], Ralph Süptitz[1,2], Margitta Uhlemann[1], Annett Gebert[1], and Ludwig Schultz[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany

With regard to surface finishing electroplating from aqueous solutions is a very common method. It is well-known, that by superposition of homogeneous magnetic fields the deposition process as well as morphology, texture and magnetic properties of deposits can be changed due to Lorentz force induced convection. Additionally, it has been shown that non-homogeneous magnetic fields are able to increase deposition rates dramatically due to the Magnetic field gradient force acting on paramagnetic ions. However, effects of magnetic gradient fields on deposit properties are still not well investigated, although interesting results due to interaction of Lorentz force and Magnetic field gradient force might be expected.

Hence, this work is focused on externally applied, well-defined magnetic gradient fields and their impact on deposition behavior and deposit properties. It has been found that structured deposits and significant diversification of roughness and grain structure can be observed. Effects of the involved magnetic forces are considered in order to propose a structuring mechanism, which bases on magnetically induced local convection.

MM 31.35 Wed 17:15 P5

Ab initio simulation of coherent phonons in BN-nanotubes — •Bernd Bauerhenne, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

BN nanotubes are isostructual to carbon nanotubes with boron and nitrogen atoms occupying the even and odd sublattices, respectively. An intense ultrashort laser pulse excites the electronic system to very high temperatures, whereas the ions remain close to their initial state. The ensuing laser-induced processes of electronic origin include bond softening, phonon frequency changes (hardening or softening), and the excitation of coherent phonons. We study these processes by means of large-scale molecular dynamics simulations based on density functional theory, including levels of excitation where the nanotube breaks. Our results show a strong radial breathing mode, increasing in amplitude with the laser-induced electronic temperature. We also determine the damage threshold.

MM 31.36 Wed 17:15 P5

Nano-morphology of optoelectronic circuits exploiting focused ion beam lithography — Selcuk Zorlu[1], •Hideyuki Maki[1,2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TUM Garching, Germany — [2]Department of Applied Physics and Physico-Informatics, Keio University, Hiyoshi, Yokohama, Japan

We present studies on the nano-morphology of optoelectronic circuits by exploiting a focused ion beam (FIB) lithography in combination with an electron beam microscope. To this end, lamellas of optoelectronic circuits are fabricated in a cross-beam (FIB and e-beam) microscope. The lamellas are side-cuts of the circuits, and they give access to the vertical structure of the semiconducting, metal, or organic layers. The presented method allows analyzing interpenetrating networks of vertical, optoelectronic two-terminal circuits.

MM 31.37 Wed 17:15 P5

Pore lattice deformation of silica nanochannels (SBA-15) during uptake and release of solid and liquid argon — •Daniel Rau[1], Dirk Wallacher[2], Gerald Zickler[3], Patrick Huber[1], and Rolf Pelster[1] — [1]FR 7.2 Experimentalphysik, Universität des Saarlandes, Germany — [2]Helmholtz Zentrum Berlin, Germany — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität / University of Leoben, Austria

We have studied the structural change of cylindrical, hexagonally ordered silica nanopores (SBA-15) as a function of their filling with solid and liquid argon, respectively. Sorption isotherms were measured at 71.5 K (solid) and 81.5 K (liquid). Simultaneously the material was characterized via small-angle-X-ray-scattering (SAXS) using synchrotron radiation at the Hasylab (DESY/Hamburg). In this way we are able to evaluate the deformation of the pore lattice during adsorption and desorption.

MM 31.38 Wed 17:15 P5

Synthesis of ZnO core spike particles as composite fillers with a high throughput method — •Sebastian Wille, Tönjes Koschine, Christoph Chluba, Stefan Freitag, Yogendra Kumar Mishra, and Rainer Adelung — Funktionale Nanomaterialien, CAU Kiel

ZnO core spike particles are typically micro particles covered with nanoscopic spikes. They show advanced properties compared to conventional fillers like roundish particles and short fibers. An example is a very strong mechanical interlocking behaviors. This property together with its hardness makes this material very interesting for compounds with enhanced mechanical properties. In addition ZnO has very interesting electric and electronic properties, which make the range of possible applications for composites containing ZnO core spike particles very wide. In order to use ZnO core spike particles as filler for bulk materials, considerable amounts are necessary. A problem during the oxidation based synthesis of such particles using Zn-powder as source material is the separation of the single Zn-particles, which is necessary for oxygen supply, for avoiding sinter processes and allowing the nanoscopic spikes to grow. We introduce simple processing routes found as solution for this problem. Large amounts of microscopic Zn-powder can be converted to ZnO core spike particles with a total size from nanometers up to a couple of micrometers. Furthermore by changing the growth parameters it is also possible to modify the particle shape.

MM 31.39 Wed 17:15 P5

DFT studies of clusters and nanowires in external fields — •Marcus Beck, Gary Klindt, Manuel Matt, and Peter Nielaba — University of Konstanz, Department of Physics, 78457 Konstanz, Germany

Density functional theory (DFT) studies on the stability and structural properties of small clusters and nanowires are performed. One point of interest is the arranging of diverse Si nano clusters. We use external electrostatic fields for ordering purposes of these clusters by polarization effects. We further investigate the $Al_{13}H$ cluster with distorted icosahedral formed Al_{13} which has several isomers with different positions of the hydrogen atom. We analyze the effects of electrostatic and magnetic fields on these systems in order to explore the possibility to switch the isomers by external fields. The geometrical configuration of monoatomic Au nanowires and the structural change due to an external electric field is also part of our investigations. Distances, angles and binding energies are influenced by the field and therefore breaking of the nanowire is more likely. These changes may influence the conductance of the wire substantially which we study using the non equilibrium Greens function formalism (NEGF).

MM 31.40 Wed 17:15 P5

Laser-assisted atom probe tomography of self-organized surface layers — •Andreas Stoffers and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany

The availability of femtosecond lasers facilitates the analysis of new material classes by atom probe tomography. Pulsed-laser atom probe tomography (PLAP) has the potential to give even structural and chemical information of biological and organic materials at an atomic scale. In order to explore the possibilities of analyzing nanometric materials, we have chosen the model cases of polyelectrolyte multilayers (PEM) and self assembled monolayers (SAM). PEMs are adsorbed step by step as a multilayer of poly-anions and poly-cations at the apex of sharp gold tips. SAMs are also adsorbed in a self-assembling process at the apex of sharp gold tips, but offer only a limited volume for analysis. By means of laser-assistance it is indeed possible to chemically analyze different PEMs and SAMs. In all cases the mass spectra are complex, characterized by peaks of multiple fractions of different molecular mass. Since these molecular species are very similar for the studied polymer types, it is hard to distinguish the organic molecules from the time-of-flight spectrum. However, different polymer-types might be distinguished based on the intensity ratio between characteristic mass peaks. In addition, a 3D reconstruction of a fluorinated SAM will be presented to demonstrate the ability of getting structural information of the alignment and distribution of the oligomeres.

MM 31.41 Wed 17:15 P5

Spin wave modes in magnetic nanostructures as seen by Ferromagnetic Resonance — •Sven Stienen, Ralf Meckenstock, Christoph Hassel, Jürgen Lindner, Nathalie Reckers, and Michael Farle — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

Micromagnetic simulations using the 3D Object Orientated Micromagnetic Framework (OOMMF) software were performed for a permalloy (Py) stripes arranged in a the form of crosses. In difference to most previous work, we apply a small time-dependent magnetic field with a fixed frequency (10GHz) to simulate the microwave field used in ferromagnetic resonance (FMR). Different spin wave excitations like the uniform, edge and not-aligned modes can be identified and visualized in time and space. In the simulation an external in-plane angular dependent magnetic field is varied between 0mT and 400mT yielding spectra as in the experimental ferromagnetic resonance. These simulated spectra are compared to experimental spectra of structured samples. Our simulation yields visualizations of the distribution of the excitation inside the stripes thus unambiguously identifying more than 10 different modes occurring in the stripes. These simulated images and spectra are helpful to find the best conditions for locally resolved ferromagnetic resonance measurements. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB 491.

MM 31.42 Wed 17:15 P5

Phase-field Modeling of Twin Boundary Motion in Magnetic Shape Memory Alloys — •Christian Mennerich, Frank Wendler, Marcus Jainta, and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Magnetic shape memory (MSM) alloys have gained high interest in the last decade. As actuators, they provide fast response times and low energy costs in operation. When in the low temperature martensitic state, large recoverable strains (more than 6% in Ni_2MnGa-based alloys) can be achieved in these ferromagnetic hard materials by controlling the motion of twin boundaries by applying an external magnetic field.

Using a multi-phase field model of Allen-Cahn type basing on a Helmholtz free energy density formulation, the microstructure rearrangement in Ni_2MnGa is described. Order parameters, related to the different eigenstrains of the twin variants, describe their time-spatial evolution, depending on energy contributions for twin interfaces and bulk phase states (including micromagnetic and magneto-elastic energies). Assuming an isothermal setting below the Curie temperature and the martensitic start temperature, we can solve for the elastic displacement field (damped wave equation) and the volume averaged magnetization (Landau-Lifshitz-Gilbert equation using a geometric integration scheme). We show results of simulations of the reversible transformation process in single crystals, and we propose an extension of the model to polycrystalline settings. The coupled evolution of twin variants and magnetic domains is investigated in more detail, and the resulting magnetic domain structure is visualized.

MM 31.43 Wed 17:15 P5

TEM Investigations on NiMnInCo and Fe70Pd30 Ferromagnetic Shape Memory Alloys — •Burak Erkartal[1], Andriy Lotnyk[1], Viola Duppel[2], Robert Niemann[3], Christoph Bechtold[4], Christiane Zamponi[4], Sebastian Fähler[3], Ludwig Schultz[3], Eckhard Quandt[4], and Lorenz Kienle[1] — [1]Synthesis and Real Structure, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart — [3]IFW Dresden, P. O. Box 270116, 01171 Dresden — [4]Inorganic Functional Materials, CAU Kiel, Kaiserstr. 2, 24143 Kiel

NiMnInCo meta-magnetic shape memory alloys have attracted considerable interest because they can be utilized for the magnetocaloric effect. Here we focus on TEM investigations of an epitaxially grown NiMnInCo thin film sputtered on (001) oriented MgO substrate with Cr buffer layer. Besides the presence of 6M, 7M modulated martensites, structural analysis by precession electron diffraction confirm also a non-modulated tetragonal phase. EDX elemental maps recorded on a cross-section indicate defects of the Cr buffer layer at the interface. Additionally, columnar regions with lower In content were observed. Further interest was concentrated on Fe70Pd30 due to the exceptional strain in response to a variation of a moderate magnetic field. Fe70Pd30 was deposited by magnetron sputtering on (001) MgO substrates coated with different metallic buffer layers. HRTEM micrographs and diffraction patterns confirm the tetragonal single crystal growth of the Fe70Pd30 films of ~1.2 micrometer thickness. The authors thank the DFG for funding via the SPP 1239.

MM 31.44 Wed 17:15 P5

Low-temperature relaxation in NiTi-based shape memory alloys — •Joan Torrens-Serra, Daniel Salas, Eduard Cesari, and Sergey Kustov — Departament de Física, Universitat de les Illes Balears, cra. de Valldemossa km 7.5, E-07122, Palma de Mallorca, Spain

We have studied the structural changes occurring in different Ni-Ti and Ni-Ti-Fe alloys over the temperature range from 13 to 300 K by means of mechanical spectroscopy, calorimetry (DSC) and electrical resistivity measurements. Several binary and ternary alloys were used with different thermal and mechanical history, which demonstrate distinct transformation paths: B2-B19', B2-R and B2-R-B19'. Temperature dependence of the internal friction (IF) was studied over the range 90-137 kHz for different strain amplitudes from 3*10E-7 to 5*10E-5. In addition to the martensitic and intermartensitic transformations, the IF curves showed a peak at about 90 K in annealed and water-quenched samples independently of their composition which can not be detected by DSC or electrical resistivity measurements. The thermally activated nature of the relaxation has been confirmed using different measurement frequencies. Since the IF peak is observed for ultrasonic frequencies at temperatures of around 90 K, it corresponds to a new relaxation phenomenon, not reported so far in Ni-Ti family of alloys, with the activation energy of the order of only 0.01 eV. On the other hand, no relaxation is found in deformed alloys not subjected to annealing heat treatments. The origin of this relaxation may be attributed to the presence of interstitial hydrogen atoms.

MM 31.45 Wed 17:15 P5

The effect of cooling rate on undercooling of pure Sn single drop — •Bin Yang[1], Yulai Gao[2], Alexander S. Abyzov[3], Evgeny Zhuravlev[1], Jürn Schmelzer[1], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Germany — [2]Shanghai

Key Laboratory of Modern Metallurgy & MaterialsProcessing, Shanghai University, China — [3]National Science Center, Kharkov Institute of Physics and Technology, Ukraine

The cooling rate dependence of undercooling of pure Sn single drop is studied by the non-adiabatic fast scanning calorimetry in a large range of cooling rate spanning four orders of magnitude. The experimental results and theoretical analysis show that the undercooling can be obviously increased first with increasing cooling rate going over to a stage of slow increase for high cooling rates, which indicates a shelf-like dependence of undercooling on cooling rate before and after a "crossover" at higher cooling rate where two different heterogeneous mechanisms act simultaneously.

MM 31.46 Wed 17:15 P5

Computational approaches to compute interface tensions γ_{lw} and γ_{cw} for colloidal systems — •Debabrata Deb, Alexander Winkler, Peter Virnau, and Kurt Binder — Johannes-Gutenberg-Universität, Staudinger Weg 7, 55099 Mainz, Germany

On this poster we present recent efforts to calculate interface tensions γ_{lw} between liquid and wall and γ_{cw} between crystal and wall for hard spheres and the effective Asakura-Oosawa model. Wall interactions are modelled with the purely repulsive Weeks-Chandler-Andersen potential. Several approaches are tested: A method based on the anisotropy of the pressure tensor for γ_{lw}, a recent approach to compute absolute free energies proposed by Schilling and Schmid [1], and a thermodynamic integration based on slowly moving the system away from the bulk towards the confined state.

[1] T. Schilling and F. Schmid, J. Chem. Phys **131** (23), 231102 (2009)

MM 31.47 Wed 17:15 P5

Determination of the pressure activation volume via the deformation of nanocrystalline PdAu-samples with different shear-compression-ratios — •Christian Braun and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

The recently introduced miniaturisation of the shear-compression-specimen [1] allows the mechanical testing of small samples such as inert gas condensed nanocrystalline materials via a dominant shear-deformation. The stress-strain-curve and further parameters as strain components or hydrostatic pressure P are calculated by FEM-simulations based on the experimental force-displacement-diagram. By means of a variation of the shear-angle, it is possible to vary the shear-compression-ratio and the hydrostatic pressure P in the deformation zone. This permits the determination of the differential quotient $\partial\sigma/\partial P$ which is necessary to calculate the pressure activation volume Δv_P given as $\Delta v_P = \frac{\partial\sigma}{\partial P}\Delta v_\sigma$, where Δv_σ is the shear activation volume obtained from stress-strain-curves taken at different strain rates [2]. On this poster we present first simulation results for the expected variation of P for different shear angles as well as first experimental findings measured at nanocrystalline $Pd_{90}Au_{10}$-samples with an average grain diameter of about 10 nm.

[1] M. Ames, J. Markmann, R. Birringer, Mater. Sci. Eng. A 528, 526 (2010), [2] A.S. Argon, Strengthening Mechanisms in Crystal Plasticity, OUP (2007)

MM 31.48 Wed 17:15 P5

In situ tensile testing of single crystal Au nanowires — Bahne Kapelle[1], •Burkhard Roos[1], Gunther Richter[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Max-Planck-Institut für Metallforschung, Stuttgart

The mechanical properties of nanoscale metals differ from those of macroscale samples, especially the increasing strength with decreasing sample size. In this work, the stress-strain behavior of single crystalline Au nanowires with diameters between 40 and 200 nm are studied using an instrumented tensile stage in an SEM. The wires are transferred from the growth substrate to the tensile stage without deforming them using a micromanipulator. Displacements are applied by a piezoelectric based actuator while forces are measured with a capacitive MEMS device. All tested wires show an initial elastic regime with a slope of around 68GPa, which is reversible on unloading. This is followed by a gradual onset of plasticity and eventually by fracture after a plastic strain of 1 to 3%. The failure stresses, which reach up to 1.2GPa, confirm the trend that smaller samples have higher flow stresses than bulk materials. Investigations of the failed wire segments, which were transferred subsequently to a TEM grid, confirm the size-dependent deformation mechanisms observed during in situ TEM tensile testing, namely that deformation proceeds by partial dislocation motion rather than full dislocation motion below a critical size of approximately 180 nm.

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Effect of hydrogen on the multiplication of dislocations in cold-rolled palladium — •Hans Peter Barth, Yuzeng Chen, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

According to a novel defectant (defect acting agents) concept (R. Kirchheim, IJMR (Z. Metallkde) 100 (2009) 483 and Acta Materialia 55 (2007) 5129 and 5139), the solute-defect interaction in materials can reduce defect formation energies. In the present work, the influence of hydrogen (defactant) on the multiplication of dislocations in cold-rolled palladium is studied. Palladium is used as a model system because it offers a sufficient hydrogen solubility and fast hydrogen diffusion. Well annealed palladium was electrochemically charged with different amounts of hydrogen ($\leq$1at%) and subsequently cold-rolled to a certain deformation degree. Pure palladium was also cold-rolled to the same deformation degree for comparison. Afterwards, the hydrogen was electrochemically uncharged from the deformed samples. Dislocation densities were studied by means of XRD and electromotive force (EMF) measurements during hydrogen recharging. Compared to pure palladium, X-ray profiles of samples charged with hydrogen prior to deformation exhibit more significant Bragg peak broadening, indicating higher dislocation densities. EMF measurements confirm the conclusion from the XRD measurements. Both methods suggest hydrogen can facilitate the multiplication of dislocations in palladium. Apart from the above results, a new experimental setup for in-situ EMF measurements during tensile tests will be shown.

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Die Bonner Positronen Mikrosonde - ein vielfältiges Werkzeug für die Materialforschung — •Niels Lennart Raeth[1], Olga Herdt[1], Meng Liu[1], Benedikt Klobes[1], Matz Haaks[1], Karl Maier[1] und Christoph Hugenschmidt[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nußallee 14-16, 53115 Bonn — [2]FRM II und Physik Department E21, Technische Universität München

Die Bonner Positronen Mikrosonde (BPM) erzeugt einen fein fokussierten Positronenstrahl mit einstellbarem Strahldurchmesser von 1 - 200 μm und besitzt ein integriertes Rasterelektronenmikroskop (REM). Proben können so lateral hochaufgelöst mit den Methoden der Positronenannihilationsspektroskopie (PAS) untersucht werden und man erhält Zugang zur detaillierten Messung von Plastizität und Defektdichten verschiedenster Materialien.

Instrumentell ist eine Weiterentwicklung der BPM im Bereich der Strahlfokussierungs- und -justagesysteme geplant. Zudem soll die BPM um die Möglichkeit zur ortsaufgelösten Messung der Positronenlebensdauer ergänzt werden.

Der aktuelle Fokus der Forschung liegt auf schweißbaren Aluminiumlegierungen der Systeme AA5xxx und AA6xxx. Besonderes Interesse gilt hier der Defektkonzentration direkt an der Schweißnaht und in der angrenzenden Wärmeeinflusszone, vor allem im Hinblick auf eine PAS-basierte Schadensvorhersage für geschweißte Aluminiumwerkstoffe.

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Tailoring the mechanical properties of nanocrystalline fcc metals: A Molecular Dynamics study on the effects of twins and miscible solutes on deformation processes — •Jonathan Schäfer, Alexander Stukowski, and Karsten Albe — TU Darmstadt, Darmstadt, Germany

For the presence of twins, a strengthening effect of nanocrystalline metals has been reported in experiment and simulation. For the case of miscible solutes, little is known about their effect on the structure and properties of nanocrystalline metals.

We present a comparative atomistic study on the effect of twins on the deformation behavior of nanocrystalline Cu and Pd. A new analysis method based on an automated Burgers circuit is applied, which allows us to analyze the dislocation interactions with twin planes and grain boundaries, and to directly measure dislocation, stacking fault, and twin boundary densities as functions of strain. We show, how a strengthening or softening effect of twins depends on the properties of a given fcc material i.e. its generalized planar fault energies.

For the case of Pd, we additionally show, how miscible solutes (Au) influence the behavior of our nanocrystalline structures in the elastic and plastic regime and why this depends on the distribution of the

solutes. Here, samples are alloyed using a hybrid MD-MC method sampling the semi-grandcanonical ensemble. The automated Burgers search is applied as well and allows us to quantitatively compare the slip processes and planar faults as a function of composition and relaxation state.

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Dynamics of small strain plasticity within the framework of a phase-field model — •Jan Höhn[1], Daniel Schneider[1], Alexander Vondrous[2], and Britta Nestler[1,2] — [1]Institute for Reliability of Components and Systems, Karlsruhe Institute of Technology — [2]Institute of Materials and Processes, Karlsruhe University of Applied Science

A small strain plasticity model, based on the principles of continuum mechanics, was incorporated into a phase-field model for polycrystalline material systems in order to investigate the influence of plastic deformation on the change of the free energy. As a first approach, the Prandtl-Reuss model was implemented consisting of an associated flow rule in combination with the von Mises yield criterion and a linear isotropic hardening approximation. The fundamental set of equations is derived from an energy density functional and the numerical solution method is described. Simulations with simple loads on microstructures were performed illustrating the dynamic evolution of the stress and plastic strain by solving the momentum balance and by using a radial return mapping algorithm, respectively. An outlook on the long-term objectives of the new phase-field model is given ranging from applications to crack propagation, recrystallisation and annealing processes.

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Examination of stress drops due to grain boundary motion in nanocrystalline PdAu-samples — •Michael Davis, Christian Braun, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

The miniaturized shear-specimen [1] allows one to examine the mechanical behaviour of nanocrystalline materials under dominant shear deformation. Due to the localisation of the plastic deformation in the gauge section, this samples geometry is particularly useful to study shear-stress driven grain boundary migration [2]. MD simulations predict a stick-slip-like deformation manifesting as stress drops in the force-displacement-diagram. In order to elucidate stick-slip behaviour, we probe the shear deformation in the gauge with high resolution optical displacement measurements. [1] M. Ames, J. Markmann, R. Birringer, Mater. Sci.Eng. A 528, 526 (2010), [2] J. W. Cahn, Y. Mishin, A. Suzuki, Acta Mat. 54,4953 (2006)

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Mechanical characterization of chromium-based adhesion layers for hydrogenated amorphous carbon coatings — •Christoph Schmid, Jens Schaufler, Verena Maier, Karsten Durst, and Mathias Göken — Department of Materials Science and Engineering, Institute I, University Erlangen-Nürnberg, Germany

Hydrogenated amorphous carbon (a-C:H) coatings show unique properties, such as high hardness, low coefficients of friction and chemical inertness, which make them suitable for the application as wear protective coatings. At this the interfacial adhesion strength between steel substrates and the coating is a crucial point which often limits the reliability of coated components in high load applications. On an industrial scale metallic adhesion layers are a common technique to achieve a well adherent a-C:H coating. In this work, two chromium-based adhesion layers for a-C:H coatings with different adhesion qualities and a total thickness of less than 1 micron were investigated. By carrying out in-situ bending tests on FIB-milled micro-cantilevers in a SEM, the interface fracture strength between the adhesion layer and the a-C:H coating were determined quantitatively. Furthermore, nanoindentation tests on small angle cross sections (SACS) of the coating systems revealed information about the mechanical properties in terms of Hardness and Young‘s modulus. Performing auger-electron-spectroscopy on the SACS differences in the chemical gradients for the investigated adhesion layers can be found. With these results a correlation between the interfacial adhesion strength with the chemical composition and the mechanical properties of the coating systems can be given.