MM 15: Poster Session

Time: Monday 18:00–20:00 Location: Poster E

MM 15.1 Mon 18:00 Poster E

Precipitate Formation in Fe-Cu Systems investigated by Computer Simulations — •Johannes Zeman[1], Kai Kratzer[1], David Molnar[2], and Axel Arnold[1] — [1]ICP, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]IMWF, Universität Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany

At temperatures above 300°C, copper-alloyed bcc-iron relatively quickly shows the formation of copper nanoprecipitates strongly affecting its mechanical properties. We investigate the kinetics of this phase transition qualitatively and quantitatively, using a vacancy-based atomistic kinetic Monte-Carlo simulation [1]. At high supersaturations, we find that Ostwald ripening is the dominant process, while at low supersaturations, nucleation determines the overall time scale of the transition. The time-temperature- transformation analysis [2] on the whole range of temperatures therefore requires the combination of brute force simulations and forward flux rare event sampling [3]. Our simulations show good agreement with the Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory.

[1] P. Binkele: Atomistische Modellierung und Computersimulation der Ostwald-Reifung von Ausscheidungen beim Einsatz von kupferhaltigen Stählen, PhD thesis, University of Stuttgart (2006)

[2] E. J. Mittemeijer: Fundamentals of Materials Science, p. 426, Springer, Heidelberg (2011)

[3] R. J. Allen, C. Valeriani, and P. Rein ten Wolde: Forward flux sampling for rare event simulations, J. Phys. Condens. Matter 21 (2009)

MM 15.2 Mon 18:00 Poster E

Grain boundary chemistry in nickel alloys applied in 700°C coal-power plant — •Miriam Magdalena Lange[1], Sergiy Borodin[1], Michael Spiegel[2], and Frank Uwe Renner[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Department for Interface Chemistry and Surface Engineering, Düsseldorf, Germany — [2]Salzgitter Mannesmann Forschung GmbH, Duisburg, Germany

Nickel-based alloys are highly interesting materials for application in the new technology of 700°C coal-power plants. Compared to conventional power plants the temperature is increased from 600°C to 700°C at a pressure of 350 bar. During first tests under flue gas atmosphere and pressurized steam the nickel-based alloys showed significant grain boundary sulfidation. The grain boundary chemistry before and after sulfidation under high-temperature working conditions of specific variants of Alloy 617 and corresponding model casts have been investigated by means of Auger Electron Spectroscopy (AES), accompanied by conventional surface analysis. Understanding the mechanisms of grain boundary sulfidation as a result of a specific grain boundary chemistry of these materials can help to improve their corrosion resistance by grain boundary engineering. Initial results on the investigation of grain boundary chemistry of Alloy 617 before and after sulfidation will be presented.

MM 15.3 Mon 18:00 Poster E

Projection potentials and total energy convergence in the KKR method — •Rudolf Zeller — IAS-3, Forschungszentrum Juelich

Although the full-potential Korringa-Kohn-Rostoker Green function method yields accurate results for many physical properties, the convergence of calculated total energies with respect to the angular momentum cutoff is usually considered to be less satisfactory. This is surprising because accurate single-particle energies are expected if they are calculated by Lloyd's formula and because accurate densities and hence accurate double-counting energies should result from the total energy variational principle. It is shown how the concept of projection potentials can be used as a tool to analyse the convergence behaviour. The key factor blocking fast convergence is identified and it is illustrated how total energies can be improved with only a modest increase of computing time.

MM 15.4 Mon 18:00 Poster E

Mechanical and magnetic properties of Fe-Cu and Ni-Cu nanocomposites — •Tomáš Káňa[1] and Mojmír Šob[2,1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Brno, Czech Republic — [3]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Using ab initio calculations, we predict theoretical tensile strength of Fe-Cu and Ni-Cu nanocomposites consisting of Fe or Ni nanowires embedded in the Cu matrix along the [100] direction; simulation of tensile and compressive tests is performed along this direction. We find that the presence of Fe nanowires enhances the maximum deformation in tension and diminish the maximum stress in compression. On the other hand, Fe nanowires do not affect the maximum stress in tension. The preferred mutual magnetic ordering of the nanowires is antiferromagnetic (AFM) one with parallel orientation of all spins in each individual nanowire. The energy gain of this AFM ordering decreases with increasing distance of Fe nanowires. Ni nanowires in Cu matrix do not affect the maximum deformation but enhance the maximum stress in tension. No magnetic ordering of Ni nanowires was found.

MM 15.5 Mon 18:00 Poster E

Cation -Anion interactions, Noncentrosymmetry vs Centrosymmetry : A first-principles study — •Abhishek Kumar Mishra[1], Kenneth V. Poeppelmeier[2], and Umesh V. Waghmare[1] — [1]Theoretical Sciences Unit, J Nehru Centre for Advanced Scientific Research, Bangalore-560064, INDIA — [2]Departments of Chemistry, Northwestern University, Evanston, Illinois, 60208-3113

Materials with non-centrosymmetric (NC) structure posses different technologically important physical properties such as piezoelectricity, ferroelectricty and pyroelectricity due to their symmetry dependent properties. These properties make them find applications in different fields viz. burglar alarms, pollution monitors, thermal detectors, multifunctional devices, photonics technology. Several interesting interrelationships occur between the symmetry-dependent properties and that is why these materials are of special interest in materials chemistry.

We present a theoretical study of structure-property correlation in noncentrosymmetric KNaNbOF5 and centrosymmetric CsNaNbOF5, based on first principles calculations followed by subsequent comparison with experiments. We have worked on stability, electronic and polar properties of these structures and on their solid solutions. Electronic density of states calculations reveals specific bands responsible for breaking of centrosymmetry in these structures. Using Berry phase method we have calculated values of polarization and also reported electronic dielectric constant values.

MM 15.6 Mon 18:00 Poster E

Investigation of thermal properties of Si1-xGex melts under microgravity conditions — Bernd Damaschke[1], •Yuansu Luo[1], Suresh M. Chathoth[1], N.V. Abrosimov[2], M. Czupalla[2], and Korand Samwer[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Leibniz Institut für Kristallzüchtung Berlin

Investigation of thermal properties of Si1-xGex melts has been planned on board of the international space station (ISS) under microgravity and electromagnetic levitation (EML) conditions, where the absence of gravity-driven convection and segregation of the components allows precision measurements for the thermal expansion, surface tension and viscosity as function of temperature. The semiconductor alloy crystals for the ISS experiments were prepared by Czochralski growth. For the preparation, parabolic flights (PF), which provided a microgravity condition for ca. 20s, were carried out using the samples Si1-xGex made by arc-melting (x=0, 0.25, 0.5, 0.75 and 1.0). Preliminary data of their density, thermal expansion and surface tension in the melt and undercooled state were obtained. The density shows a non-ideal behavior with x and the highest value occurs at x=0.5, indicating a strong ordering tendency. We report about sample characterization and the status of the project concerning the ISS experiments. The initial results demonstrate that the melts of these alloys can be successfully processed in the MSL-EML facility for precision measurements on board the ISS. We thank DLR and Novespace for the PF campaigns and the MUSC team for the help with experiments. Financial support from DLR project 50WM0541 and 50WM1036 is gratefully acknowledged.

MM 15.7 Mon 18:00 Poster E

Molecular Dynamic Simulation of atomic deposition between MnAs cluster — •Andreas Rühl and Christian Heiliger — I. Physikalisches Institut, Justus Liebig Universtität Giessen, D-35392 Giessen, Germany

MnAs is a promising ferromagnetic material for magnetoelectronic devices, in particular as nano-scaled clusters, providing a great tunability concerning the shape and position. We investigate hexagonal MnAs clusters which are separated by a metal. Such structures could be produced by using a FIB (focused ion beam) two disconnect two touching MnAs clusters and to deposit a metal between them. Before doing a molecular dynamic simulation of the problem at hand one needs to find the corresponding effective potentials describing the interaction of the MnAs surface with the metal atoms. We did this by fitting the chosen potential model, here the Embedded Atom Method, to a set of ab initio data (Force Matching Method).

MM 15.8 Mon 18:00 Poster E

Ab initio calculation of phonon tunneling in Au/Vacuum/Au by atomistic Green's function formalism — •Saeideh Edalati Boostan, Michael Czerner, Michael Bachmann, and Christian Heiliger — 1I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Although phonons require matter to exist recent experimental and theoretical papers have shown that phonons can cross vacuum gaps of a few angstroms wide. This effect is called phonon tunneling [1,2,3]. In this work we calculate phonon tunneling in Au(111)/Vacuum/Au(111) by using an ab initio approach based on density functional theory. The interactions between atoms are modeled by inter atomic force constants, which are calculated by the abinit software package in the harmonic approximation. These inter atomic force constants are used as an input into an atomistic Green's function (AGF) method in order to calculate the transmission function of the system as a function of the thickness of the vacuum gap.

[1] Igor Altfeder et al., Phys. Rev. Lett. 105, 166101 (2010)
[2] Mika Prunnila and Johanna Meltaus, Phys. Rev. Lett. 105, 125501 (2010)
[3] D. P. Sellan et al., Phys. Rev. B 85, 024118 (2012)

MM 15.9 Mon 18:00 Poster E

Mechanical analysis of amorphous solids with large amplitude oscillatory spectroscopy (LAOS) — •Stefanie Finkhäuser, Carsten Mahn, and Konrad Samwer — 1.Physikalisches Institut, Georg-August Universität Göttingen

In the presence of mechanical fields glassy materials are known to reveal many interesting phenomena. One of them is a crossover from a linear behavior in stress-strain dependency to a nonlinear behavior. To investigate this crossover in detail we use dynamic mechanical excitation with large amplitudes and different frequencies. The sample is excited with a sinusoidal stress whose amplitude is large enough to lead to nonlinear strain-responses. The FFT-analysis of these nonlinear responses contains higher harmonic contributions. These can give further insight into interactions among local plastic events, which lead to the nonlinear response. We will show first results on PMMA and amorphous PdCuSi.

Financial support by the DFG SFB937 is thankfully acknowledged.

MM 15.10 Mon 18:00 Poster E

Charge and Spin transport in Turbostratic Graphene and Graphene Nanoribbons — •Nils Richter[1], Sebastian Schweitzer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Jakoba Heidler[4], Xinliang Feng[3], Petr Ostrizek[1], and Mathias Kläui[1,2,4] — [1]4Institut für Physik, Johannes Gutenberg Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]FB Physik, Universität Konstanz, Universitätsstr. 10, D-78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, German — [4]SwissFEL, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Single Layer Graphene (SLG), which is a simple 2D honeycomb lattice made of carbon atoms, is still one of the most promising materials for scientific research and moreover for nanoelectronic and spintronic devices. Here we present electrical and magnetic transport in two highly interesting Graphene allotropes: Turbostratic Graphene (TG) and Graphene Nanoribbons (GNR). TG is a stack of Graphene where every layer is rotated by a certain angle. Nevertheless it retains important properties similar to SLG due to electronical decoupling. High mobilities of 10^5 cm^2/Vs were measured in TG discs [1] and spin injection in a non-local spin valve [2] has been investigated. Measurements with atomically precise GNR [3] indicate quantum transport behaviour at low temperatures and theory predicts magnetic edge states [4].

[1] Y. Hernandez et al., (under review). [2] N. Tombros et al., Nature 448, 571 (2007). [3] Cai et al., Nature 466, 470-473 (2010). [4] O. Yazyev et al., Phys. Rev. Lett. 100, 047209 (2008)

MM 15.11 Mon 18:00 Poster E

Stability Analysis of Intrinsic Colloidal Quasicrystals: A Recipe for Designing Quasicrystals — •Erdal Celal Oğuz and Michael Schmiedeberg — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

A big advantage of studying colloidal quasicrystals is that individual particle positions are directly observable (eg. by using video-microscopy) and therefore real-space information is accessible. Another advantage is that the interaction between the colloidal particles in principle can be fine-tuned. In this work, we investigate the ground state (T=0) stability of colloidal quasicrystals by minimizing the lattice sum. For this purpose, we develop lattice summation techniques for quasicrystals with 5-, 8-, 10- and 12-fold rotational symmetry. Subsequently, we minimize the potential energy with respect to particle coordinates for various pair interaction potentials with two length scales. Our goal is to find suitable isotropic interaction potentials that lead to stable quasicrystalline order.

MM 15.12 Mon 18:00 Poster E

Symmetry and electronic structure study of a predicted carbon structure — •Torsten Weissbach, Silvia Bahmann, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, D-09596 Freiberg

A new metastable structure for carbon, which is presented in by the authors in another contribution, was predicted theoretically. It consists of structural building blocks of diamond and graphite and exhibits tubular pores, similar to the carbon foam class of structures. Here, we investigate the symmetry of the structure and its reflection in the calculated electron and phonon band structure. Like graphite, this new carbon structure exhibits a band crossing at the Fermi level and zero band-gap. Compared to graphite, the deformation stability is enhanced by the links between the graphene planes.

MM 15.13 Mon 18:00 Poster E

Characterization of Pulsed CNT Field Emitters for Medical Imaging — •Daniela Leberl[1,2], Bernhard Hensel[2], and Sandro Francesco Tedde[1] — [1]Siemens AG, Corporate Technology, Erlangen, Germany — [2]Center for Medical Physics and Engineering, University Erlangen-Nuremberg, Erlangen, Germany

Cold electron sources for X-ray applications would be beneficial for reduced acquisition time and improved image quality compared to thermionic emitters, today's state of the art. Carbon nanotubes (CNTs) are a promising material for field emission applications due to the high aspect ratio and high electrical and thermal conductivity. For motion-free 3D image acquisition, short electron pulses of many individual sources are necessary. Thus it is important to investigate the field emitter characteristics and stability under pulsed conditions.

Here we report on electrical characterization of multi-walled CNTs grown by thermal chemical vapour deposition on stainless steel substrates. We studied the dependence of the IV characteristics and emitter stability on pressure, pulse-on time and duty cycle. All investigations have been carried out on samples with high field emission currents up to 126 mA (220 mA/cm^2) and extremely long lifetimes up to 200 cumulative hours.

We found out that the emitter degradation is an important parameter for the application in medical X-ray systems. We discuss potential degradation mechanisms and present the correlation with threshold field and field enhancement factor, calculated with the Fowler-Nordheim theory of field emission.

MM 15.14 Mon 18:00 Poster E

Stacking faults in fcc Iron: The Influence of Magnetism — •Ivan Bleskov, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

The stacking fault energy is a critical parameter that defines the type of plasticity mechanism in austenitic high-Mn steels, which are char-

acterized by a combination of enhanced formability and strength. A common concept for its description is the generalized stacking fault energy (γ-) surface, which describes the sliding of one part of a perfect crystal against the other. It provides the energy paths and barriers, which the system needs to overcome to form an intrinsic stacking fault (ISF). The goal of the present work is to study the influence of magnetism on the topology of the γ-surface. To avoid the influence of chemical effects, we have focused the investigation on pure fcc Fe. Density functional theory has been used for calculations of different magnetic (non-, ferro- antiferro-, and paramagnetic) structures. The paramagnetic state, which is closest to reality, was approximated by the disordered local moments (DLM) realized within the coherent potential approximation. Changing to magnetically ordered structures the γ-surface is strongly altered. The effects are stronger for ferro- than for antiferromagnetic configurations. The nonmagnetic γ-surface, however, is in the relevant region in very good agreement with DLM, and therefore may be used to reduce the complexity in future ISF calculations.

MM 15.15 Mon 18:00 Poster E

Investigation of the loading state dependent fracture behaviour of nanocrystalline PdAu — •Christian Braun and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

Numerous experiments exhibited that nanocrystalline materials with a mean grain size in the range of 10 to 20 nm behave different in compression and tension testing, in agreement with molecular dynamic simulations. However, investigations with other loading conditions between these two limiting cases are still scarce.

We used the miniaturized shear compression specimen (m-SCS) to study the mechanical response of nanocrystalline PdAu samples under different loading states by varying the shear angle. Since the deformation of the m-SCS samples is constrained to a cross section of 0.1 mm^2, it becomes possible to in-situ observe plastic shear and/or crack nucleation and propagation using light microscopy. Additional, post mortem REM-analysis of the fracture surfaces is carried out. We present results for specimens with shear angles of 45° and 60°. Although, upon loading a specimen, the difference in the hydrostatic pressure is small between this two sample geometries, they show a completely different behaviour: while for the 45° specimens a ductile deformation up to 20% strain is observed, the 60°-samples show brittle fracture in the transition regime from elastic to plastic deformation.

MM 15.16 Mon 18:00 Poster E

Shear compression specimens - a new approach to study the pressure and normal stress dependence of plasticity — •Christian Braun, Patrick Marx, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

The mechanical behaviour of several materials which are currently in the focus of research, like nanocrystalline metals or metallic glasses, exhibits a compression-tension-asymmetry, i.e. yielding depends on the loading condition. While this compression-tension-asymmetry of yielding is well examined in simulations, experiments are still rare for various reasons: On the one hand the ductility of these materials is often limited in a tensile test and on the other hand there are only a few involved methods to probe other loading states than pure compression and tension.

A new approach to study the pressure or normal stress dependence of plasticity is exploiting shear compression specimens (SCS) with different shear angles. The sophisticated data analysis of these experiments based on FEM-simulations allows to extract all components of the stress and strain tensor and so to relate the state of stress to the observed yielding behaviour. We present a feasibility study with stainless steel as reference material to demonstrate the potential of this testing method.

MM 15.17 Mon 18:00 Poster E

Relationship between enthalpy relaxation and shear modulus relaxation below and above the glass transition of metallic glasses — •Yuriy Mitrofanov[1,2], Andrey Makarov[3], Vitaly Khonik[3], Andrew Granato[4], Dave Joncich[4], and Svetlana Khonik[5] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Solid State Physics, State Technical University, Voronezh, Russia — [3]Department of General Physics, State Pedagogical University, Voronezh, Russia — [4]Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA — [5]Centre for Joint Research, State University, Voronezh, Russia

Despite decades-long investigations of the enthalpy relaxation in metallic glasses, its nature remains unclear. To understand the nature of the enthalpy relaxation near Tg, we used an approach, that is based on the interstitialcy theory. We derived a simple and testable expression for the heat flow (enthalpy relaxation rate) occurring upon heating of the glass at a constant rate. This heat flow is mostly determined by the shear moduli of the glass and the parent crystal. The shear modulus of the glass is defined by the concentration of frozen-in interstitialcy-like defects (atomic configurations with two atoms sharing the same potential well). The relaxation law describes both, the exothermic heat flow below Tg and endothermal heat flow above Tg and reflects a generic connection between the elastic properties of the glass and the parent crystal. An extensive check of the derived heat flow law for temperatures near the glass transition showed good agreement with the experiments performed on two Pd-based metallic glasses.

MM 15.18 Mon 18:00 Poster E

Time dependent development of decorated grain boundaries of severely plastically deformed Al by liquid Ga — •mehrnoosh naderi, martin peterlechner, gerhard wilde, and sergiy divinskiy — Institute of Material Physics, University of Muenster, Germany

Fast liquid penetration into the grain boundary network of a polycrystalline solid is observed for different metallic or ceramic couples. Yet, the detailed mechanism as well as morphological features or the kinetics of the penetration process are not well understood. Recent models relate the liquid penetration process to the mechanical properties of the grain boundaries. In order to investigate the importance of defect structures and residual stresses at grain boundaries for the liquid penetration kinetics, the penetration behavior of liquid Ga along fine grains of polycrystalline Aluminum produced by High Pressure Torsion was studied at room temperature. Scanning Electron Microscopy (SEM) and the so-called Automated Crystal Orientation Mapping (ACOM) technique that measures the orientations in a transmission electron microscope (TEM) have been used for this study. The development of decorated grain boundaries was investigated by SEM and the thickness of Ga layer at grain boundaries was obtained less than 1.5 nm from ACOM data as well. The results are discussed with respect of the underlying mechanism that drives liquid penetration into the grain boundary network.

MM 15.19 Mon 18:00 Poster E

Rational Tuning and Thermodynamic Characterization of Lithium Silicides as Electrode Materials for Lithium Ion Batteries — •Thomas Gruber and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics,Leipziger Str. 23, 09596 Freiberg, Germany

Li_xSi is a promising anode material for lithium ion batteries due to its high specific energy density. There are several known stable phases with different Li/Si ratio. The main goal of our investigation is to support an understanding of the charging and discharging processes, which are directly related to the Li^+ transport. For practical usage of Li_xSi in lithium ion batteries a proper understanding of the thermodynamical behavior of the material is required. The Gibbs free energy can be determined from the calculation of the phonon dispersion, which depends on pressure. We have calculated the isotropic thermal expansion of Li_7Si_3 and the non-isotropic thermal expansion of LiSi. This gives access to the thermal expansion coefficients, speci*c heat and other thermodynamical data. Our theoretical results are then compared to experimental data measured on these compounds.

MM 15.20 Mon 18:00 Poster E

Understanding the protein-inorganic crystal interaction in bioinspired syntheses — •Annalena Wolff[1], Idir Yahiatene[1], Walid Hetaba[2], Nadine Mill[1], Marco Wissbrock[3], Stefan Loeffler[2], Katrin Eckstädt[1], Norbert Sewald[3], Peter Schattschneider[4], and Andreas Hütten[1] — [1]Uni Bielefeld, Fakultät für Physik — [2]TU Wien, Institut für Festkörperphysik — [3]Uni Bielefeld, Fakultät für Chemie — [4]TU Wien, Service Center für Elektronenmikroskopie

Bioinspired syntheses have sparked great interest in the past years. Recent studies showed that proteins, involved in nanoparticle formation within natural systems, can be used to influence materials, not known to occur within these systems. The engineering process however remained elusive. Here, cobalt ferrite nanoparticles were synthesized using c25-mms6, a short synthetic version of a protein linked

to nanoparticle formation in magnetotactic bacteria. The polypeptide allows the formation of stoichiometric, shape specific nanoparticles, which cannot be achieved under similar conditions by conventional chemical synthesis. The particles were studied at different times during nanoparticle growth using TEM, HRTEM and EELS to gain a better understanding of the engineering process. The polypeptide - inorganic crystal interaction was studied in FCS measurements. The results suggest that the polypeptide adsorbes onto the (111) face of the particles,reduces its surface energy, and allows the formation of hexagonally shaped nanoparticles. The polypeptides can be easily removed after the growth process which is advantageous for applications.

MM 15.21 Mon 18:00 Poster E

Influence of the sputter parameters on surface segregation and silver ion release properties of reactively sputtered Ag/TiOx nanocomposites — •Jian Xiong[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Ulrich Schürmann[2], Lorenz Kienle[2], Frank Lehmann[3], and Franz Faupel[1] — [1]Institute for Materials Science-Multicomponents Materials, CAU Kiel, Kaiserstr. 2, 24143, Kiel, Germany — [2]Institute for Materials Science- Synthesis and Real Structure, CAU Kiel, Kaiserstr. 2, 24143, Kiel, Germany — [3]Dept. of Prosthodontics, Propaedeutics and Dental Materials, CAU Kiel , Arnold-Heller-Str. 3, 24105, Kiel, Germany

Reactive sputtering of silver/titania nanocomposites is potentially attractive for antibacterial coatings based on the release of silver ions. Previous studies on such coatings showed strong segregation of silver towards the surface. Surface segregation leads to rapid depletion of the Ag in humid invironment and prevents tailoring of the release properties. In this work, the influence of sputter parameters on the morphology and subsequent silver ion release properties of reactively sputtered silver/ TiOx nanocomposites was investigated. It was observed that silver surface segregation is largely independent of the oxygen partial pressure used in the sputtering process and that - unlike in nonreactive sputtering of TiOx - even sputtering of pure TiOx barriers at moderate deposition rates is not sufficient to prevent the strong surface segregation. Surface segregation is significantly reduced for silver filling factors below a critical silver content of 9% and can be further be reduced by deposition of TiOx barriers with high sputtering rates.

MM 15.22 Mon 18:00 Poster E

Influence of transition-metal alloying on the electro-chemical properties of (Li)$FePO_4$ as cathode material for Li-ion batteries — •Hamid Reza Hajiyani, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

One of the central challenges in increasing the performance of Li-ion batteries is the optimization of cathode aterials. The candidate compounds need to provide a technologically acceptable compromise of energy density, intercalation voltage, as well as structural and thermal stability during intercalation. A promising approach to achieve this goal for cathode materials based on $FePO_4$ is alloying by partly or fully substituting Fe with other transition metals (TMs). Here, we use high-throughput density-functional theory (DFT) calculations in order to investigate $LiM_yN_{(1-y)}PO_4$ compounds in the olivine structure. In particular, we determine the formation energy for various stoichiometric of different TMs M and N. Systematic screening across the 3d TM allows us to identify alloying trends with bandfilling and atomic size. For each binary TM phosphate we consider different levels of Li intercalation. Based on these DFT calculations we estimate the energy density, the volume expansion during intercalation, the intercalation voltage, and the thermal stability with respect to oxidation. Our calculations indicate that the energy density of the binary transition metal phosphates increase with bandfilling while the thermal stability of the compounds decreases.

MM 15.23 Mon 18:00 Poster E

Cluster expansion study of Ni–Pt alloys — •Martin Leitner, David Reith, and Raimund Podloucky — Department of Physical Chemistry, University of Vienna

The Cluster expansion (CE) is a state-of-the-art tool for exploring the configuration space of multi-component systems with the accuracy of density functional theory (DFT) calculations. Based on the figure set of a converged CE Monte-Carlo (MC) simulations are performed in order to derive temperature dependent phase stabilities.

This CE+MC approach – as implemented in the UNCLE package [1] – is applied to study the Ni–Pt alloy system, for which the formation of ordered phases at low temperatures is under debate. DFT studies focussed on three ordered phases, namely $NiPt_3$ and Ni_3Pt with $L1_2$ structure and NiPt with $L1_0$ structure. A CE study predicted an additional stable Pt-rich phase of $NiPt_7$ composition, which was not confirmed by recent DFT studies and experiment. A further DFT study predicted a Ni-rich Ni_3Pt phase with $D0_{22}$ ordering to be energetically more favorable than the $L1_2$ structure.

Based on DFT calculations performed with VASP an extensive CE+MC study was done for the whole composition range. The results will be critically compared to the existing data. Furthermore, calculated short range order intensities are compared to very recent X-ray Photon Correlation Spectroscopy (XPCS) experiments in the Ni-rich regime.

Supported by FWF, project nr. F4110 (ViCoM).

[1] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

MM 15.24 Mon 18:00 Poster E

DFT studies of the lattice thermal conductivity of thermoelectric materials — •René Moser[1], Mingxing Chen[2], and Raimund Podloucky[1] — [1]Department of Physical Chemistry, University of Vienna — [2]Department of Physics, University of Wisconsin-Milwaukee

Thermoelectric materials are of technological and scientific interest because of their ability to convert a temperature gradient directly into electric energy. The efficiency of this process is defined by the figure-of-merit $Z = TS^2\sigma/\kappa$ which contains the Seebeck coefficient S, the electrical conductivity σ and the thermal conductivity κ at a given temperature T. A large Z is achieved by a large S and a small κ, which properties one tries to optimize. The total thermal conductivity $\kappa = \kappa_{el} + \kappa_{ph}$ is the sum of the electronic contribution κ_{el} and the phonon mediated lattice thermal conductivity κ_{ph}. Here we focus on the first-principles modelling of κ_{ph} by a density functional (DFT) theory approach for the electronic structure and phonon properties in combination with Boltzmann's transport theory. Results are presented and discussed for a selection of thermoelectric materials.

Supported by FWF, project nr. P24380.

MM 15.25 Mon 18:00 Poster E

Matrix-induced in situ growth of plasmonic Au nanoparticles for biological sensor devices — •Philipp Naujok[1], Christian Katzer[1], Peter Michalowski[1], Frank Schmidl[1], Markus Westerhausen[1], Gabriele Schmidl[2], Robert Mueller[2], Jan Dellith[2], Christa Schmidt[2], Jacqueline Jatschka[2], and Wolfgang Fritzsche[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena - Helmholzweg 5, D-07743 Jena, Germany — [2]Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, D-07745 Jena, Germany

In the past years different methods such as wet chemical synthesis where established to fabricate metal nanoparticles which can be used in bio-photonic sensor devices. In order to overcome the multiple preparation steps and typical solution based problems like aggregation of particles, new in-situ methods of preparation directly on the substrate surface are highly favoured. The authors present a novel in-situ method of fabricating crystalline gold nanoparticles by self-organization using two different thin film matrices ($YBa_2Cu_3O_{7-\delta}$ and $SrTiO_3$). We will show that the interaction of nanoparticles and thin film matrix allows controlling not only the size (between 10 and several hundreds of nm) and distribution of gold nanoparticles but also their shape. A subsequent dissolution process of the matrix enables us to extract the nanoparticles to receive immobilized crystalline particles directly on a substrate surface. The spectral characterization of those particles will be presented based on microspectroscopy. [1] C. Katzer et al., J. Nanopart. Res. 14, 1285 (2012)

MM 15.26 Mon 18:00 Poster E

Coulomb drag in monolayer graphene — •Jonathan Lux — Institut für theoretische Physik, Universität zu Köln

Coulomb drag measurements provide an interesting possibility to study interaction effects between two adjacent layers. If a current is driven in one of the layers, called the active layer, via Coulomb interaction, momentum can be transferred to the other layer, called the passive layer. This can induce a voltage drop in the passive layer, which can be measured. The ratio of the voltage drop in the passive layer and the current in the active layer is called the drag resistance.

We have calculated the drag resistivity in MLG using Boltzmann kinetic theory, taking into the two relevant modes for both particles and holes in each layer. In the Fermi liquid (FL) regime of monolayer graphene (MLG), the drag resistivity is, up to numerical prefactors,

identical to the one in the 2 dimensional electron gas, and independent of the impurity configuration.

Near charge neutrality, Coulomb interaction is able to relax the current, due to the particle–hole symmetry of the low energy Dirac theory of MLG. This defines a new regime, which is not accessible in FLs. We found that here the result depends on the ratio of the scattering times of Coulomb and impurity scattering. In the very clean limit, when the impurity density reaches zero, the drag resistivity assumes an universal finite value, although the individual conductivities diverge.

MM 15.27 Mon 18:00 Poster E

Stacking fault energy of a binary Fe_xMn_{1-x} mixed crystal calculated by combing cluster expansion and DFT — •Sebastian Schwalbe, Torsten Weissbach, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, D-09596 Freiberg

Physical properties like mechanical stability and ductility of highly alloyed steels play an important role in material science. The stacking fault energy (SFE) [1] is a powerful instrument for the characterization of such systems. Both cluster expansion (CE)[2] and the calculation of the SFE can be expressed with the Ising-model formalism. The CE relies on the division of the lattice into different geometrical clusters, and calculating their total energy (e.g. using LAPW[3]). This enables the calculation of total energies for mixed crystal models. The aim of this work is to exploit the combination of DFT and CE for the special case of SFE computation.

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[3] Blaha, P.,Schwarz, K., Madsen, G. K. H., Kvasnicka, D., Luitz, J.: WIEN2k, Techn. Universität Wien, Austria, 2001.

MM 15.28 Mon 18:00 Poster E

Investigation of possible solid state reaction in the Fe-Al-O system based on density functional theory. — •Lilit Amirkhanyan, Torsten Weissbach, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, D-09596 Freiberg

Particles in a metallic melt can be filtered out using ceramic filters, which are often based on corundum. From experiments it is known that new phases (e.g. $FeAl_2O_4$) can be formed during the filtering process. We study several solid state reactions using density functional theory (DFT) calculations. By varying the volume and calculating the corresponding total energy we obtained the equation of states for α-Al_2O_3, metastable κ-Al_2O_3, Fe_2AlO_4, $FeAl_2O_4$, $FeAlO_3$, FeO.

This allows to discuss possible phase formation mechanisms based on energy differences obtained from DFT. In particular we will focus on the possibility to form hercynite $FeAl_2O_4$.

MM 15.29 Mon 18:00 Poster E

High Throughput Preparation and Scanning of a Complex Perovskite Oxide Library for Light-driven Electrocatalysis — •Helge Stein, Andreas Blumenstein, Julius Scholz, Jörg Hoffmann, and Christian Jooss — Institut für Materialphysik, Friedrich-Hund Platz 1 37077 Göttingen, Deutschland

With respect to development of novel materials for sunlight driven photocatalysis, high-throughput preparation and characterization methods are preferable because of the broad chemical search space. We have designed a system for the screening and production of ternary and quaternary oxide compounds in order to find promising compositions which have a well-matched electronic band structure and sufficient complexity to enable a multi-step charge transfer reaction. As a model system we have prepared a multi-component La-Sr-Fe-Co (LSFC) oxide library for testing oxygen evolution under sunlight irradiation. This system is mostly of perovskite type and shows a broad doping ability as well as a complex electronic structure. The samples were deposited on glass using an ink-jet printing technique with nitrate precursors. By post-annealing in air for 4 hours at 480°C Oxide phase formation was performed. Electrocatalytic measurements were made by high throughput cyclic voltametry in darkness and under illumination. The Crystallographic structure and surface morphology of the samples was determined by x-ray and SEM techniques.

MM 15.30 Mon 18:00 Poster E

Grain boundary free energies from the reweighted path ensemble — •Jutta Rogal and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The grain boundary free energy and mobility are important quantities in describing grain growth and thus the evolution of the microstructure in polycrystalline materials. In this study we use transition path sampling (TPS) to investigate the transformation of one particular grain orientation into another via the migration of a grain boundary within a Lennard-Jones system. The trajectories describe the entire transition including the initial formation of the grain boundary. By reweighting the path ensemble it is then possible to extract the free energy as a function of any arbitrary order parameter and thus determine the grain boundary free energy at various temperatures. Since all trajectories in the path ensemble are true dynamical trajectories of the system the path ensemble also contains information about the mobility as well as the migration mechanism of the grain boundary.

MM 15.31 Mon 18:00 Poster E

High-Performance LFP Thin Film Electrodes — •Frank Berkemeier, Mathias Köhler, Lea Lüken, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm Str. 10, D-48149 Münster

Thin films of lithium iron phosphate (LFP) are prepared by reactive ion beam sputtering, with a thickness between 50 and 500 nm. The structure and morphology of the layers is investigated by X-ray diffraction measurements and transmission electron microscopy, while their electrochemical properties are characterized by means of cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and the galvanostatic intermittent titration technique (GITT). It is observed that the electrochemical performance of the layers strongly depends on the preparation conditions during sputtering. Thus, using optimum deposition conditions, a reversible capacity of 104 $mAh\,g^{-1}$ is found, and a cycling stability at 1 C rate which allows to perform more than 1700 cycles before observing a capacity loss of only 20%. In addition, the lithium diffusivity is measured by EIS and GITT, and is found to be in the range of 10^{-13} cm^2s^{-1}. This quite high diffusivity value is attributed to the strong texture of the deposited LFP films.

MM 15.32 Mon 18:00 Poster E

V_2O_5 thin films for Li-ion battery applications — •Tobias Gallasch, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Ion beam sputtered V_2O_5 thin films (thickness 10 nm - 200 nm) are investigated electrochemically via cyclic voltammetry and chronopotentiometric measurements. Within these measurements a capacity of about 400 mAh/g for reversible lithium storage is reached. In addition, Li^+ diffusion coefficients are determined by different approaches and compared to each other.

Structural changes between as-prepared, partially charged and cycled thin films are evaluated in detail by HR-TEM and EELS and the lithium signal is evaluated, directly, depending on the state of charge.

Thus, in this work the link between Li intercalation processes and morphological changes is worked out combining modern techniques of electrochemistry and analytical TEM.

MM 15.33 Mon 18:00 Poster E

Percolated Pd thin films for hydrogen sensors — •Magnus Hamm, Stefan Wagner, and Astrid Pundt — Institut für Materialphysik, Friedrich-Hundt-Platz 1, D-37077, Goettingen, Germany

It's easy accessibility and high chemical energy density makes hydrogen interesting as a future energy carrier. In addition hydrogen allows a CO2 free energy production by its reaction with oxygen to water. However one major drawback of hydrogen is its dangers when in contact with oxygen. At concentrations in the regime of 4% to 94% hydrogen is highly flammable and explosive, which makes it difficult to store and transport. Out of these reasons effective hydrogen sensors are needed for a large scale hydrogen energy network. In this work the up-to-date development of hydrogen sensors is presented and compared to a new type of thin film palladium sensor. We deposited thin Palladium films on Sapphire substrates. Later the film was fractured by Joule heating. This leads to a percolated surface which shows large resistivity effects when contacted with hydrogen. The Sensor shows good reversibility at slow reaction and decay times in the minute range. However the resistivity changes up to 6000% when contacted with hydrogen and the minimal detection limit lies at 10-20 mbar, values which both exceed other hydrogen sensors. Financial support by the DFG via PU131/9 and SFB602 is gratefully acknowledged.

MM 15.34 Mon 18:00 Poster E

Electrochemical Hydrogenography of Palladium, Magnesium

and Titanium — •Jara Kürschner and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Germany

The storage of hydrogen in metals is a safe and volumetrically desirable way. Rapid determination of the hydrogen concentration c_H in gas-phase loaded metal thin films can either be done by resistivity or transmission measurements as the electronic structure of the metal changes during hydrogenation. Since some years, the optical transmission T is applied in a technique named "Hydrogenography" to determine the hydrogen concentration in thin alloy films. A linear relationship $c_H \propto \ln(T/T_{Metal})$, as predicted by the Lambert-Beer law, is commonly assumed although it holds the assumption of the free lattice gas model.

The model does neither imply non-homogeneous hydrogen distributions as occurring during phase transitions of many metal-hydrogen systems, nor stresses, plastic deformation and film buckling which are often arising in clamped thin films.

This study analyzes the dependency between optical transmission and hydrogen concentration for clamped and quasi-free palladium, magnesium and titanium thin films. Via electrochemical hydrogen loading, the hydrogen concentration is independently controlled and the applicability of the Lambert-Beer law can be tested.

Financial support by the DFG via PU131/9 and PU131/10 is gratefully acknowledged.

MM 15.35 Mon 18:00 Poster E

Influence of hydrogen on Ta(110) surfaces — •Sebastian Schleicher, Sara Wanjelik, and Mathias Getzlaff — Heinrich-Heine-Universität

Hydrogen in metals has attracted a lot of attention in the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamental point of view.The goal of our investigations is a study of hydrogen absorbtion in a Ta(110) crystal. Careful cleaning of the Tantalum surface is essential as preparation for any measurement. The cleaning procedures are similar to those already discussed in various publications, involving flashing to high temperatures close to the melting point to remove H and O absorbates, and heating in an oxygen atmosphere to remove residual carbon impurities. Measurements are performed by means of scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) in ultra-high vacuum conditions.

MM 15.36 Mon 18:00 Poster E

Second-Harmonic Generation in Silver Nanorod Arrays — •Fabian Patrovsky[1], Vera Hoffmann[1], Philipp Reichenbach[1], Andreas Hille[1], René Kullock[2], and Lukas M. Eng[1] — [1]Institute of Applied Photophysics, TU Dresden, Germany — [2]Department of Experimental Physics 5, University of Würzburg, Germany

Second-harmonic generation (SHG) in metal nanoparticles is a promising new field combining nanotechnology with nanooptics [1]. Previous studies excellently proved the SHG effect of single nanoparticles attached preferentially to nonconductive surfaces. Similar to Raman scattering [2], the SHG efficiency can be considerably increased when coupling two such nanoantennas in the optical near-field region [3].
In the present study we investigate the generation of second-harmonic radiation from silver nanorod arrays as a function of different geometric parameters (volume, rod length, distance) including also the angle of incidence. Correlations between linear and nonlinear optical properties are found.

[1] M. D. McMahon et. al. Physical Review B 73, 041401(R) (2006) [2] P. Olk et. al. Nano Lett. 7 (6), pp 1736-1740 (2007) [3] R. Jin et. al. J. Am. Chem. Soc. 127, 12482 (2005)

MM 15.37 Mon 18:00 Poster E

Electric field gradient at the A site in selected MAX phase solid solutions studied with perturbed γ-γ angular correlation — •Christoph Brüsewitz[1], Daniel Jürgens[1], Ulrich Vetter[1], Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

MAX phases represent a class of complex carbides and nitrides which combine prominent features of both metals and high performance ceramics. They are good electric and thermal conductors, thermal and mechanical shock resistant, and easily machinable. Perturbed γ-γ angular correlation (PAC) offers, using implanted ^{111}In as probe atom, an insight into the local environment of the probes at the A-sites of many MAX phases by studying the electric field gradient (EFG). Starting with Ti_2AlC, the variation of the EFG caused by systematic replacement of half of M atoms with V, A atoms with In, and X atoms with N is investigated. Additionally, these results are compared with the EFG of the corresponding end members V_2AlC, Ti_2InC, and Ti_2AlN. The existence of a single phase is confirmed through XRD. This work is supported by the DFG under contract HO 1125/19-2.

MM 15.38 Mon 18:00 Poster E

Electrochemical lithiation/delithiation analysis of silicon as anode material for lithium-ion batteries — •Gibaek Lee[1,2], Stefan L. Schweizer[2], and Ralf B. Wehrspohn[1,2] — [1]Fraunhofer Institute for Mechanics of Materials — [2]Martin-Luther-University Halle-Wittenberg

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 lithiation/delithiation, resulting in mechanical disintegration of electrode and rapid capacity fading. Therefore, relaxation of the stress caused by the expansion and contraction of Li-Si alloy materials is important to obtain a good cyclability.

In this study, we prepared oriented silicon nanowire arrays (SiNWs) on n-type silicon substrate by metal-assisted chemical etching in aqueous HF solution containing AgNO3. The electrochemical properties of the SiNWs electrode were systematically investigated. The material characteristics have been analyzed by Cyclic voltammetry (CV), XRD, SEM and TEM. The performance of SiNWs electrode have been examined by galvanostatic charge/discharge cycling. In addition, to compare the battery cycle behavior of the different structure of silicon anode material, we have investigated the characteristic and transformation of other types silicon anode such as black silicon and macroporous silicon obtained by reactive ion etching (RIE) etching and electrochemical etching, respectively.

MM 15.39 Mon 18:00 Poster E

Phase-field crystal approach to model interfaces and crystal nucleation in binary alloys — •Muhammad Ajmal Choudhary[1], Julia Kundin[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth. — [2]Institut für Angewandte Physik, Universität Tübingen, D-72076, Tübingen.

In general, the properties of a material are strongly related to the nucleation and patterning of its microstructure. Phase-field crystal (PFC) modeling is widely used to address the nucleation and microstructure evolution phenomena. We used a binary alloy system to study the equilibrium properties of liquid-solid interfaces as well as the nucleation barriers. We proposed the method of determining interfacial energies for a curved liquid-solid interface by stabilizing the circular solid seed in the surrounding liquid phase as well as the liquid droplet in the solid phase for various seed sizes in a finite system. We also derived the free energy barriers for the nucleation and investigated the system size effects on the equilibrium properties of liquid-solid interface and nucleation barriers. Furthermore, we compared the simulation results with the existing theories as well as the predictions based on the classical nucleation theory.

MM 15.40 Mon 18:00 Poster E

DFT calculation of cleavage energies and γ-surfaces in Mo_2BC hard coatings — •Tobias Klöffel[1], Sandra Korte[2], and Bernd Meyer[1] — [1]Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg — [2]Lehrstuhl für Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg

The unusual combination of high stiffness and moderate ductility makes Mo_2BC a very interesting material for application as hard protective coating of cutting tools. In order to obtain more detailed insights into the properties of dislocations and plastic deformation in Mo_2BC we have calculated the γ-surfaces for several crystallographic crystal cuts using density functional theory. For many simple fcc and bcc metals a detailed atomistic understanding of dislocation properties has been gained on the basis of Peierls-Nabarro models and calculated γ-surfaces. However, such an approach has not been attempted yet for more complex compounds such as Mo_2BC. Here, the first results on the shape and properties of the γ-surfaces will be discussed. It will

be shown that it is not possible to conclude from the decohesion energy which crystallographic plane will be the active plane for plastic deformation. Finally, the results for the critical Peierls stress and the preferred shear planes will be compared to experimental observations in mechanical tests on micrometer-sized Mo_2BC pillars.

MM 15.41 Mon 18:00 Poster E

First-principles calculations and kinetic Monte Carlo simulations of screw dislocation motion in dilute W alloys — •Leili Gharaee[1], Alexander Stukowski[2], Jaime Marian[3], and Paul Erhart[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Lawrence Livermore National Laboratory, Livermore, California

Tungsten is being considered as a candidate material for structural applications in fusion reactors. The performance of the pure material is, however, limited by a high ductile-to-brittle transition temperature (DBTT), which can be lowered by alloying for example with small amounts of Re. These alloys are, however, not suitable for applications in fusion environments due to neutron activation of Re, which motivates the search for alternative alloys. The present work addresses the potential of dilute W-Ti alloys to accomplish a lowering of the DBTT. To this end, we have studied the elastic properties of intrinsic defects and substitutional alloying agents in body-centered cubic tungsten as well as their direct interaction with screw dislocations using density functional theory. In this fashion we determined deformation volume tensors and interaction strenghts for each of these entities. The thus obtained information was subsequently employed to parametrize a kinetic Monte Carlo model for screw dislocation motion that takes into account the elastic interaction between dislocation segments and point defects. This approach enabled us to study systematically the effect of various defects on the mobility of screw dislocations as a function of shear, temperature, and defect density.

MM 15.42 Mon 18:00 Poster E

Highly ordered metal nanowire arrays as active substrate of SERS — •Yong-Tae Kim[1], Stefan L. Schweizer[1], and Ralf. B. Wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg — [2]Fraunhofer Institute for Mechanics of Materials

Metallic nanostructured materials have fascinating potential applications in the nanodevices, especially as an efficient substrate for surface-enhanced Raman scattering (SERS). In SERS, as one of the most promising optical sensing techniques, the Raman signal can be amplified by several orders of magnitude by the use of metallic nanostructure substrates. 1-dimensional metallic nanostructures show some advantages associated with their anisotropic architecture and enable to be employed as highly active substrate of SERS.

The key obstacle for the practical use of SERS devices is the lack of robust and facile fabrication strategies for reproducible SERS substrates with stable enhancement. Although traditional SERS substrates such as colloidal nanoparticles, metal islands, and fractal film provide significant SERS enhancement, the well ordered 1-dimensional metallic SERS substrates with reproducible and deterministic geometries are needed for detection of trace level molecules in gases or liquids.

In this study, single- or multi-segmented 1-dimensional highly ordered metallic nanowire arrays composed of nickel, silver, and gold have been fabricated by simple pulsed electrodeposition in the pores of anodic aluminum oxide (AAO). Various 1-dimensional metallic nanowire arrays with different diameter, length, and sequence of metal segments are tailored as active substrate of SERS.

MM 15.43 Mon 18:00 Poster E

Auf $Pt/peO - TiO_2/Ti$ **basierender** H_2**-Generator** — •Ömer Cakabay, Mhamed El Achhab und Klaus Schierbaum — Heinrich-Heine-Universität Düsseldorf, Institut für Experimentelle Physik der kondensierten Materie, Abteilung für Materialwissenschaft, Universitätsstraße 1, 40225 Düsseldorf

Wir berichten über die Entstehung einer elektromotorischen Kraft an Platin-bedeckten plasmaelektrolytisch oxidierten Titanfolien, die bei Raumtemperatur von einem Wasserstoff-Sauerstoff-Gemisch beströmt werden [1]. Bei diesen Bedingungen kann man entweder eine Spannung $V \leq 465$ mV zwischen Platin und Titanfolie messen, wobei der Platinkontakt gegenüber dem Titankontakt positiv ist, oder einen Kurzschlußstrom; wir haben Proben hergestellt, bei der die Kurzschlußstromdichte Werte von bis zu 20 mA/cm^2 aufweisen kann, wenn der Wasserstoffgehalt 3,5 Vol-% in Luft beträgt und die Probe in einer Stömungsapparatur mit einem Gasstrom von 100 ml/min überströmt wird. Stromabwärts beobachtet man eine Verringerung der Wasserstoffkonzentration und eine Erhöhung der Feuchtekonzentration, die die katalytische Oxidation von H_2 am Platin beweist. In dem Beitrag werden diese Messungen quantitativ ausgewertet; sie bestätigen auch das einfache physikalisch-chemische Modell dieses Chemogenerators, das in [1] vorgeschlagen wurde. Wir berichten auch über präparative Möglichkeiten zur Erhöhung der Stromdichte dieses Chemogenerators.

[1] K. Schierbaum and M. El Achhab, Phys. Status Solidi A 208, No. 12, 2796-2802 (2011) / DOI 10.1002/pssa.201127400

MM 15.44 Mon 18:00 Poster E

Influence of defects on hydride formation in thin metal films — •Marc Waninger, Sönke Schmidt, and Astrid Pundt — Instiute of Material Physics, University of Goettingen, Friedrich-Hund-Platz 1, D-37077 Goettingen, Germany

Some metals are capable of absorbing hydrogen in the interstitial sites of the lattice. Additionally, microstructural defects (vacancies, grain boundaries, dislocations etc.) offer sites for hydrogen with binding energies, different from that of the interstitial sites[1].On the one hand hydrogen preferentially dissolves at these defects and they act as hydrogen traps. On the other hand, the incorporation of hydrogen in defects changes their mobility and reduces their repulsive interaction. For dislocations this is known as HELP mechanism, which is important for the hydrogen embrittlement.

In this study, indentation and argon ion bombardment are used to artificially create defects in thin metal films. Indentation is done by using the tip of an atomic force microscope (AFM) and results in dislocation rich volumes underneath the indent. Ar-ion bombardment results in a high density of interstitials and vacancies. These defect rich films are loaded with hydrogen from the gas phase. It is investigated by in-situ AFM, resistivity measurements and x-ray diffraction, if and how the defects affect the hydrogenation behavior of the films.

This research is kindly supported by SFB602, B12 and DFG PU131/9.

[1] A. Pundt, R. Kirchheim, Annual Review Materials Research*36* (2006) 555 - 608.

MM 15.45 Mon 18:00 Poster E

Large Scale Atomistic Simulations on Nanostructure Evolution — •Jeffrey Kelling[1,2] and Karl-Heinz Heinig[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, TU-Chemnitz, Chemnitz, Germany

The Kinetic Metropolis Lattice Monte-Carlo (KMC) method is a means of performing atomistic simulations of self-organization processes in solids at by far larger scales than those accessible via Molecular Dynamics (MD). GPUs currently provide the highest peak processing performance regarding both cost and energy consumption. We present a GPU implementation of KMC achieving up to two order of magnitude higher performance than a sequential reference implementation on a single core of a modern CPU. This enables atomistic simulations at experimental spatiotemporal scales.

MM 15.46 Mon 18:00 Poster E

Simulation of the elastic properties of nanomechanical resonators — •Kristian Scholz, Daniel Mutter, Markus Ring, Ralf Schmid, Martin Vögele, and Peter Nielaba — Physics Department, University of Konstanz, Germany

The oscillation behaviour of Silicon nanomechanical resonators in the form of doubly clamped beams is investigated by Molecular Dynamics simulations using the Stillinger-Weber interaction potential. After setting up the initial structure using a diamond lattice and a (2x1) symmetric dimer surface reconstruction, the end points of the beams are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the beams. Besides varying the size of the beams, the effects of temperature, external stretching fields and cavities are explored. The results show a decrease of the oscillation frequencies and an increase of the damping coefficient with rising temperature, a strong increase of the frequencies with external stress (stretching), a decrease of frequencies with length and an increase of the damping coefficient when adding cavities to the structures. It is also possible to observe the dissipation of energy from the collective oscillation of the beams into thermal energy of the degrees of freedom of the constituting atoms. Other materials (e.g. NiTi memory alloys) and membranes are explored as well. In order to explore quantum effects in the low temperature regime Path Integral Monte Carlo simulations are performed.

MM 15.47 Mon 18:00 Poster E

Advanced electronic structure calculations of transparent conducting oxide materials — Hemant Dixit, Rolando Saniz, Dirk Lamoen, and •Bart Partoens — CMT and EMAT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

Transparent conducting oxides (TCO) constitute a unique class of materials which combine two physical properties together - high optical transparency and high electrical conductivity. TCOs are widely used in commercial applications such as liquid crystal displays, touch-screen devices, solar cells etc. Thus it is imperative to search for high performance novel TCO materials system. An accurate description of electronic band structure lies at the heart of advanced materials design. Despite of the success demonstrated by ab-initio density functional theory in describing ground state material properties, the key physical property of TCO i.e. the band gap, is poorly described with the standard local density approximation or generalized gradient approximation. Here we will discuss the electronic band structure of prototype TCO materials using advanced electronic structure methods, namely, the state of the art GW approximation and Tran-Blaha modified Becke-Johnson potential scheme. The results obtained for the key physical properties namely the band gap and electron effective mass are discussed along with the position of the 'd' orbitals in the electronic band structure. Such a systematic comparison provides useful insights into the electronic band structure of complex oxide systems and also suggests a recipe for high-throughput materials design.

MM 15.48 Mon 18:00 Poster E

Atom Probe Tomography of Polyelectrolytes and Metall Compounds — •Martin Lütkemeyer — Institut für Materialphysik, Münster, Germany

Laser Assisted Atom Probe Tomography (LA-TAP) with femtosecond lasers has the potential to give chemical and structural information of organic materials like polymers at an atomic scale. We are able to measure and identify poly(acrylic acid) and poly(allylamine hydrochloride) which are deposited on the apex of tungsten tips. The deposition is done by the Layer by Layer technique, in which the tungsten tips are consecutively dipped into poly-anion and poly-cation solutions so that a polyelectrolyte multilayer (PEM) system is build. This procedure enables us to investigate metallic nanoparticles in a new way with the LA-TAP by simply embedding them into the PEM's by dipping the polymer coated tungsten tips into a solution of colloidal nanoparticles. However, due to complex mass spectra and difficult evaporation behaviors of both PEM-matrix and nanoparticles the measurement and reconstruction of these tips is challenging. To demonstrate that it is indeed possible to get chemical and structural information of those materials at such a small scale with the LA-TAP, reconstructions of Au-nanoparticles embedded in PEM's, and corresponding composition profiles and mass spectra will be presented.

MM 15.49 Mon 18:00 Poster E

Origin of the p-type and n-type conductivity in novel spinel transparent conducting oxides ZnX_2O_4 — Mozhgan Amini, Hemant Dixit, Rolando Saniz, Dirk Lamoen, and •Bart Partoens — CMT and EMAT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

ZnM_2O_4 (M=Co, Rh, Ir) spinels are one of the promising p-type transparent conducting oxide (TCO) systems, while $ZnAl_2O_4$ (Gahnite) is considered as a possible n-type TCO. We report the formation energy of acceptor-like (in ZnM_2O_4) and donor-like (in $ZnAl_2O_4$) defects using first principles calculations with an advanced hybrid exchange-correlation functional (HSE06) within the density functional theory (DFT). For ZnM_2O_4 spinels we present results for the cation vacancy and the antisite defect, which are the leading sources of disorder in the spinel structures. We also discuss the band alignments in these spinels.

Further, we have investigated the formation energies of intrinsic defects in $ZnAl_2O_4$ which include the Zn, Al and O vacancy, and the antisite defects: Zn at Al site (Zn_{Al}) and Al at Zn site (Al_{Zn}). The antisite defect Al_{Zn} has the lowest formation energy and acts as a shallow donor, indicating possible n-type conductivity in $ZnAl_2O_4$ spinel by Al doping.

MM 15.50 Mon 18:00 Poster E

Large-area structuring of nanorod arrays by laser interference lithography — •Eric Jehnes[1], Vera Hoffmann[1], René Kullock[2], Gunther Scheunert[3], and Lukas M. Eng[1] — [1]Department of Applied Photophysics, TU Dresden, Germany — [2]Department of Experimental Physics 5, University of Würzburg, Germany — [3]Department of Physics and Astronomy, Queen's University, Belfast, UK

Metal nanorod arrays grown in anodic aluminum oxide show distinct plasmonic resonances, which can be tuned via the rod length, diameter and spacing of the rods [1,2]. However, the influence of structuring (e.g. parallel lines of rods) on the plasmonic properties has not yet been investigated. The work we present concerns the preparation of such structured arrays. To arrange the rods, laser interference lithography is used. This method is able to deliver high-quality periodic photoresist patterns with low defect densities over an area of several cm^2. To integrate the structuring process into the nanorod fabrication, lithography is combined with wet etching and physical vapor deposition. The resulting structures are expected to show new optical properties that can be used to increase the tunability of the plasmonic resonances. Hence, structured arrays find applications in optical waveguides and sensors both for the visible and near infrared range. Furthermore, our technique provides the basis for the low-cost integration of optoelectronic and storage devices based on such nanorod arrays.

[1] R. Kullock et al., Optics Express 16, 21671 (2008) [2] R. Kullock et al., J. Opt. Soc. Am. B 27, 1819 (2010)

MM 15.51 Mon 18:00 Poster E

Molecular Dynamics Simulations on the Coherency of Cu Nano Precipitates in BCC Fe — •David Molnar[1,2], Fabian Maier[1], Peter Binkele[1], and Siegfried Schmauder[1,2] — [1]Institute for Materials Testing, Materials Science and Strength of Materials (IMWF), University of Stuttgart — [2]Stuttgart Research Center of Simulation Technology (SRC SimTech), SimTech Cluster of Excellence, University of Stuttgart

The mechanical behaviour of steels is strongly related to their underlying atomistic structures which evolve during processing or thermal treatment and during their life cycles. In copper-alloyed α-iron, precipitates form within the iron matrix, especially when operated at higher temperatures of above 300°C, yielding a change of the material's mechanical properties. During growth, the approximately spherical precipitates perform a structural transition from bcc to fcc, thus increasing the incoherency between bcc matrix and precipitate. The detailed analysis of this transition on the atomistic length scale by means of Molecular Dynamics simulations is crucial with respect to sequential multiscale coupling with Phase Field Methods and Dislocation Dynamics which are able to simulate particle growth, particle coarsening and the interaction of dislocations with large obstacle fields, respectively. Structural transitions are found to nucleate in the precipitate's centre while the surface is still forced to remain bcc. We will investigate the structural transition of Cu precipitates and the effect on residual stresses and obstacle strength.

MM 15.52 Mon 18:00 Poster E

Full-Scale Modeling of APT Measurement Data — •Christian Oberdorfer, Sebastian Manuel Eich, and Guido Schmitz — Institut für Materialphysik, Münster, Deutschland

The application of simulation enables a complementary approach to the interpretation of measurement results in atom probe tomography (APT). A very first approach to APT simulation was introduced by Vurpillot et al. The approach makes use of an iterative solution of the Laplace equation on a regular grid. Atoms of a modelled field emitter structure are consecutively detached from the surface and respective ion-trajectories are calculated. Consistent with the experimental condition in which a position sensitive detector is placed in front of the emitter sample, the simulated data result in the lateral hit positions of the ions on a simulated detector plane.

The present contribution depicts recent results which were obtained from an extended simulation approach for APT. Founded on an elaborated grid of irregular shaped Wigner-Seitz cells, the potential distribution can be solved without any constraints on the possible emitter geometry. Conceivable emitter structures consist of distinguished lattice types and orientations which reflect realistic atomic distributions. Even the analysis of amorphous structures is possible. Additionally, an adaptive grid of support points allows to extend the simulation space decisively. Ion trajectories with flightlengths of about 10 cm are enabled. — The respective "TAPSim" simulation package is freely offered.

MM 15.53 Mon 18:00 Poster E

Atomistic simulation of a severe plastic deformation-

induced "high-energy" state of grain boundaries — •Lisa Neier[1], Sergiy Divinski[1], Anantha Padmanabhan[2], Martin Peterlechner[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische-Wilhelms-Universität, 48149 Münster — [2]University of Hyderabad, India

A comparison of microstructures and properties in materials subjected to the later stages of severe plastic deformation or steady-state superplastic flow indicates several unexpected similarities especially with respect to the interface response on the deformation, such as grain boundary (GB) sliding events, which lead to a suppression of dislocation activity. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle GBs in SPD-processed materials in terms of the concept of shear localization in the interfaces and choosing oblate spheroids of a few atomic diameters size as the basic units of sliding. Atomistic simulations of these special GBs are performed. In this approach, the GB is generated, oblate spheroids are defined, extra free volume is introduced, and the oblate spheroids are sheared by a given amount. After this preparation, the whole simulation box is sheared. The GB energy as a function of the extra free volume is determined and the arrangement of the (extra) free volume in the grain boundary is analyzed. The simulation data are compared with experimentally available HRTEM images via calculation of HRTEM images corresponding to simulated GBs and subsequent geometric phase analysis of the local strain fields.

MM 15.54 Mon 18:00 Poster E

Precipitate redissolution in Al-Cu-Li- alloy AA 2195 — •Judith Leese[1], Kathrin Kolotzek[1], Melanie Markgraf[2], and Ferdinand Haider[1] — [1]Universität Augsburg, 86159 Augsburg — [2]Premium Aerotec GmbH

A decrease in density of about 3 wt% for every wt% of Lithium combined with an increase in Youngs modulus of 6 % [1] made the straight path to many applications in aeronautics for Al-Cu-Li alloys. The alloy AA 2195 keeps its superior mechanical properties even at cryogenic temperatures [2]. The strength of this age hardenable Al-Cu-Li alloys is mainly controlled by volume fraction and size of the hardening precipitates like Θ', δ' and T1. Different processes during processing in industry can influence the microstructure of the peak-aged alloy via an short term heat input. The decrease in strength can be assigned to growth and dissolution reactions of the strengthing precipitates. The current study aims to resolve the microstructural processes during heat input for the commercial aluminum alloy AA 2195 at three different temperatures (250°C, 350°C and 510°C). The heating periods were varied from a few seconds to two hours. Vickers hardness measurements characterize the strength of the alloy. DSC measurements allows to monitor further kinetic reactions and TEM was used to record the correspondent changes in microstructure like size and distribution of the relevant precipitates. The combination of the different techniques prooves several reactions like dissolution and Ostwald Ripening during heating. [1] Material Science and Engineering,1980,44(2),213 [2] Journal of Materials Engineering and Performance,1998,7(5),682

MM 15.55 Mon 18:00 Poster E

Ultra thin LiPON layers as an electrolyte for solid-state thin film batteries — •Susann Nowak, Frank Berkemeier, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Despite LiPON (lithium phosphorus oxynitride, $Li_3N_x(PO_4)_{1-x}$) is widely discussed as a suitable electrolyte for all solid-state thin film batteries, there are only a few publications reporting on films that exhibit a thickness below 1 μm. Therefore, in this work we investigate the properties of LiPON films with a thickness between 50 and 500 nm prepared by reactive ion-beam sputtering of Li_3PO_4, using argon as sputter gas and nitrogen as reactive additive and the characterization of the films by temperature-dependent electrochemical impedance spectroscopy (EIS) and transmission electron microscopy (TEM). Temperature dependent measurements of dc-conductivity by EIS give a conductivity of $5 * 10^{-7}$ S/cm at 30° and an activation enthalpy of (58 ± 2) kJ/mol, and hence allow to operate the LIPON films in all-solid state batteries at room temperature, with a reasonable charge/discharge performance. Additionally, thin film batteries have been prepared by depositing a LIPON layer between two metallic electrodes (e.g. Pt and Ag), which are forming a complete electrochemical thin-film cell during the first cycle of cyclic voltammetry measurements.

MM 15.56 Mon 18:00 Poster E

Ion diffusion in lithium titanate thin films — •Fabian Wunde, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Münster

Lithium titanate (LTO) is used as an anode material in lithium ion batteries, as it reveals both, a high ionic conductivity and the capability to reversibly intercalate/deintercalate lithium ions. In our work we use rf-ion beam sputtering to prepare LTO thin films. X-ray diffraction and transmission electron microscopy show, that the layers are crystalline and exhibit a strong orientation in (111) direction, a dense structure, and smooth interfaces. These properties open the possibility to integrate the LTO thin films in all-solid-state lithium ion batteries. On the other hand, the films can be used to study fundamental material properties like lithium ion hopping rates or diffusion coefficients, which are difficult to obtain in case of powder material. In this scope, galvanostatic intermittent titration technique (GITT) is used to determine the chemical diffusion coefficient of lithium within the LTO films. Due to the thin film geometry of the samples, it is possible to reliably evaluate the GITT results via the thin film approach and to determine the lithium diffusivity as function of the lithium concentration.

MM 15.57 Mon 18:00 Poster E

Resonant Photoemission at the O1s threshold to characterize In_2O_3 single crystals — •Jörg Haeberle[1], Matthias Richter[1], Dieter Schmeisser[1], Zbigniew Galazka[2], and Christoph Janowitz[3] — [1]BTU Cottbus, Applied Physics, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Leibniz-Insitut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, 12489 Berlin Germany

We report on spectroscopic investigations on In_2O_3 single crystals. We focus on the detailed analysis of the O1s resonance profile by resonant photoelectron spectroscopy (resPES). From these we analyze the electronic structure and assign the O2p- and In5sp-state to build the valence band and the conduction band in different contributions, respectively. This is deduced from constant final statespectra on the O-KLL-Auger along the O K-edge and In $M_{4,5}$-edge and a comparison to the corresponding X-ray absorption spectroscopy data. We also identify several types of defects. A broad band of oxygen derived defects is identified in the valence band and extends throughout the gap. Small polarons are attributed to cause an anti-resonance in the constant initial states around the O1s threshold. In addition, an Auger decay separated by the O-KLL is present at O-K resonance and indicates the existence of localized charge transfer states which involves In5sp states. Finally, we are able to distinguish two different oxygen species from the resPES data. One corresponds to theintrinsic In_2O_3 structure and the other is a non-corresponding species.

MM 15.58 Mon 18:00 Poster E

Characterisation of residual stress in steel components with non-destructive evaluation methods — •Sascha Raatz[1], Farid Hendry[1], Angga Ginandjar[1], Michael Kaack[2], Peter Staron[3], Michael Hofmann[4], and Katharina Theis-Bröhl[1] — [1]University of Applied Sciences Bremerhaven, 27568 Bremerhaven — [2]Salzgitter Mannesmann Forschung GmbH, 47259 Duisburg — [3]Helmholtz-Zentrum Geesthacht, 21502 Geesthacht — [4]Forschungs-Neutronenquelle Heinz Maier-Leibnitz, 85747 Garching

In industrial application non-destructive evaluation methods are widely used to determine residual stress to prevent failure under load. Magnetic Barkhausen noise (MBN), harmonic analysis and ultrasonic are favoured due to their simple onsite applicability with portable devices. But all those techniques have different limitations and require an independent calibration by an absolute evaluation method like X-ray- and neutron-diffraction. In our study we compare all those techniques to determine the residual stress in steel components. The chosen samples are low-alloy steel pipes with different levels of a straightening process which leaves a visible helix on the surface. This helix is measurable with MBN and harmonic analysis which are sensitive on the skin of the surface. We used synchrotron- and neutron-diffraction to get absolute values in the bulk of our samples. The residual stress correlates with the MBN results, the levels of straightening and changes its value up to 400 MPa through the wall-thickness. We acknowledge funding by BMBF, DESY, FRM II and HZG. The samples were provided by our industrial partner SZMF.

MM 15.59 Mon 18:00 Poster E

Elastic-to-plastic transition: waiting time analysis of long term creep measurements — Jon-Olaf Krisponeit[1], Karina

E. Avila[2], •Sebastian Pitikaris[1], Stefan Küchemann[1], Antje Krüger[1], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Department of Physics and Astronomy, Ohio University, Athens, OH, 45701, USA

We studied the elastic-to-plastic transition of the bulk metallic glass $Pd_{77.5}Cu_6Si_{16.5}$ under uniaxially applied tensile stress. The crossover from initially elastic behavior via small plastic events to cooperative processes resulting in the emergence of macroscopic shear bands and even catastrophic failure is a very interesting phenomenon from both a materials science viewpoint and in fundamental physics. In theory, the statistic properties of avalanche-like slip events are studied intensively.

We recorded long term creep measurements (up to one week) under constant stress. Although single slip events–like activations of a shear transformation zone–are undetectable in macroscopic experiments, their cooperative avalanche-like motion is reflected in waiting time statistics. A numerical waiting time analysis was implemented and power-law behavior was found in the frequency distribution of waiting times. In addition, also power spectra have been analyzed. The results are discussed in terms of a transition from uncorrelated slip avalanches to the formation of shear bands.

We acknowledge financial support for this work by DFG via SFB 602 and FOR 1394.

MM 15.60 Mon 18:00 Poster E

Phase field modeling of interdiffusion microstructures in Ni-base superalloys — •Leslie Mushongera, Micheal Fleck, and Heike Emmerich — University of Bayreuth

The effect of the refractory element rhenium(Re) on the kinetics of coarsening in negatively misfitting ni-based superalloys during heat treatment is studied. A multicomponent phasefield model coupled with inputs from thermodynamic and kinetic databases to provide the relevant driving forces is developed. In order to realistically capture the complex nature of interdiffusion, the CMSX4 and CMSX6 superalloys with well-defined weight percent contents are analyzed.

Microstructural evolution is first studied in the presence of a lattice misfit with inhomogeneous elastic constants. Cuboidal precipitates arranged in a square array are formed. We then study the system under external load along a cubic axis. It is observed that the precipitates become anisotropic and the orientation differs depending on the sign of the applied stress. Simultaneously, we determine the mechanism by which Re reduces coarsening. It is seen that Re additions substantially reduce the rate of precipitate coarsening by keeping their shape almost cuboidal, which is the interfacial energy minimizing configuration. Re also reduces coarsening by hindering the growth of the rafts. In addition,we derive stereological measures to characterize the kinetics of coarsening.

MM 15.61 Mon 18:00 Poster E

KKRnano: Improvements in efficiency and order-N scaling for use on massively parallel computers — •Elias Rabel, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Petascale high-performance computers open completely new opportunities for the first-principles treatment of materials problems. The recently developed code KKR*nano* [1] implements the screened KKR Green's function method for DFT calculations of unit cells with thousands of atoms. It targets modern supercomputing architectures, which requires being able to utilise more than 100000 processors.

The KKR method considers multiple scattering of partial waves up to a maximum angular momentum $\ell_{\max}$. We investigate the structure of matrices with sparse block structure occuring in the treatment of very large unit cells. A distance dependent angular momentum cutoff is employed to reduce the effective matrix size with little compromise in accuracy. The special case of neglecting all partial waves at reasonably large distances leads to an $O(N)$-scaling method.

Usage of an iterative solver necessitates an appropriate preconditioning strategy. A block-circulant preconditioner has been proven to be highly effective in the case of uniform block sizes. Solution strategies for the case of the distance dependent ℓ-cutoff, where one has to deal with variable block sizes, are currently under investigation.

[1] A. Thiess *et al.*, Phys. Rev. B **85**, 235103 (2012)

MM 15.62 Mon 18:00 Poster E

Investigation of ionic surfactants capability in dispersion of multi-walled carbon nanotubes in an aqueous solution — •Maryam Khazaee[1,2], Anindya Majumder[3], Larysa Baraban[1], Joerg Opitz[1,3], and Gianaurelio Cuniberti[4] — [1]Institute for materials science and max bergmann center of biomaterials, TU dresden, 01062 dresden, germany — [2]Leibniz institute for crystal growth,12489 berlin, germany — [3]Fraunhofer institute IZFP dresden, 01109 dresden, germany — [4]Division of IT convergence engineering, POSTECH, pohang, korea

We present a comparative investigation of a dispersion of multi-walled carbon nanotubes (MWCNTs) in various ionic surfactants including three anionic and two cationic ones. The optimum sonication conditions for the dispersion of MWCNTs have been determined. Among these surfactants- Sodium dodecyl sulfate (SDS), Sodium dodecylbenzenesulfonate (SDDBS), Sodium cholate (SC), Dodecyltrimethylammonium bromide (DTAB) and Decyltrimethylammonium bromide (CTAB)- SDDBS and DTAB provided maximum and minimum dispersion susceptibility, respectively, which has a good agreement with their chemical structure properties. Dispersion efficiency of CNTs was quantified via determining extinction coefficients of these MWCNTs, derived from UV-Vis spectra. The dispersion efficiency of MWCNTs was characterized by transmission electron microscopy (TEM), UV-Vis spectroscopy and atomic force microscopy. These results serve as future guide for utilization of MWCNTs in their different applications such as nanocomposits, nanoelectronics, biosensor, etc.

MM 15.63 Mon 18:00 Poster E

Crystal growth and characterization of $Ba_8Ni_{3.5}Ge_{42.1}\square_{0.4}$ — •Stephan Pohl, Céline Grimm-Allio, Carola Dietrich, Klaus-Dieter Luther, Franz Ritter, Wolf Assmus, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

The clathrate $Ba_8Ni_{3.5}Ge_{42.1}\square_{0.4}$ possesses interesting thermoelectric properties [1]. On the one hand it features a high electric conductivity, on the other hand it has a low thermal conductivity. These properties are due to the specific crystal structure with Ba guest atoms in a Ni-Ge host lattice and might be promising towards technical applications. Neutron scattering techniques are well suited to investigate the phonon dispersions to unravel the underlying microscopic origin of the thermoelectric characteristics. However, large single crystals are required for that kind of research. Here, we show that the crystal growth of $Ba_8Ni_{3.5}Ge_{42.1}\square_{0.4}$ can be achieved by the crucible-free Czochralski pulling method. We particularly present the crystal growing achievements with a tungsten single crystal as a seed and the results of x-ray investigations on the obtained single crystals.

[1] L. T. K. Nguyen *et al.*, Dalton Trans. **39**, 1071 (2010).

MM 15.64 Mon 18:00 Poster E

Optimization of Fe/MgO/Fe Interfaces by Atom Probe Tomography — •Rabab Bahabry, Torben Boll, Ryota Gemma, and Talaat Al-Kassab — King Abdullah University of Science & Technology, Division of Physical Sciences and Engineering, Thuwal, 23955-6900, Kingdom of Saudi Arabia

As part of an emerging nanotechnology, devices based on the Tunnel Magneto-Resistance (TMR) effect have promising applications. The metal/oxide interfaces govern the magnetic properties of such multilayer structures. Hence, Atom Probe Tomography (APT) and STEM investigations help clarifying any chemical or structural inhomogeneity of these layer structures. In this paper Fe/MgO/Fe layer structures were deposited on Si-microtip coupons and W-tips by various ion beam sputtering techniques. Results obtained on several samples with differing deposition conditions utilizing the local electrode atom probe LEAP 4000 HR, which was installed recently at the King Abdullah University of Science & Technology. Results are presented and discussed in view of the influence of deposition conditions on the quality of prepared multilayer stacks.

MM 15.65 Mon 18:00 Poster E

Ab-initio prediction of the critical thickness of a coherent precipitate — Sankari Sampath, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-University Bochum

Segregation and precipitation of second phases in metals and metallic alloys are complex phenomena with a high influence on the mechanical properties of the material. Models exist that describe the growth of coherent, semi- and incoherent precipitates. One of the parameters of these models, namely the energy of the interface between matrix and precipitate is investigated in more detail in this project.

Our example is a metastable Mo-C phase, the body-centered tetrag-

onal structure, which has been observed experimentally by high-resolution electron microscopy as a semi-coherent precipitate [1]. It is assumed that it is stabilized by the precipitate interface energy. Furthermore, this interface is supposed to change from coherent to semi-coherent during the growth of the precipitate. We predict the critical thickness of the precipitate by calculating the different contributions to a semi-coherent interface energy by means of ab-initio density functional theory calculations. The parameters in our model include the elastic strain energy stored in the precipitate as well as a misfit-dislocation energy that depends on the dislocation core width and the dislocation spacing. Our predicted critical thickness agrees well with experimental observations.

[1] J.M. Pénisson, M.Bacia, M.Biscondi, Phil. Mag. A 73, 859 (1996).

MM 15.66 Mon 18:00 Poster E

Influence of Quenching & Partitioning on the Volume Fraction of Austenite Phase in Steel using X-ray Diffraction — •Karin Rüster[1], Andre Steffen[1], Michael Paulus[1], Christian Sternemann[1], Metin Tolan[1], Niko Grosse-Heilmann[2], Christian Kronholz[2], and Andreas Peters[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Benteler Tube Management GmbH, 33104 Paderborn, Germany

Steel is a common material in our daily life. Macroscopic characteristics (e.g. hardness, tensile properties) of steel are affected by the crystalline structure, i.e. austenite and martensite phase, which is changed during heat treatment. During the process of Quenching and Partitioning carbon diffuses from martensite to austenite and thereby stabilises the phase of austenite. This way a microstructure with retained austenite is produced. To investigate the material's characteristics XRD-experiments have been carried out at beamline BL9 of the synchrotron light source Delta, in Dortmund. A gain of retained austenite with increasing holding time is observed ex situ in pre-treated samples. Changes of the volume fraction of austenite during the process of heating and cooling were analyzed in situ. The stabilisation of austenite and an increase of the lattice constant both induced by the carbon diffusion was observed.

MM 15.67 Mon 18:00 Poster E

An apparatus for the synthesis of cluster-based materials — •Arne Fischer, Herbert Gleiter, and Horst Hahn — Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany

A new cluster deposition system for the synthesis of materials composed of mass-selected clusters embedded in matrices of other materials as well as cluster-decorated surfaces was constructed and first deposition experiments were performed.

The system covers a large range of cluster sizes from single atoms up to clusters consisting of several thousands of atoms and the resulting cluster beam has a narrow size distribution. During the deposition the number of clusters as well as their impact energy is well defined. Hence this approach can open pathways to a new class of materials with tailored electronic, magnetic or catalytic properties.

As a first experiment iron clusters were deposited into a silver matrix. The immiscible system Iron-Silver is a well-known GMR material. In contrast to the production via e.g. MBE where only the composition is defined with our approach we have on top control over the size of the embedded clusters. Hence it allows studying the GMR effect as a function of cluster size and density in the material. Various samples with cluster sizes from 500 to 2000 atoms and different concentrations of clusters were produced and characterized with a SQUID magnetometer. The first results look promising and prove the exceptional capabilities of our new cluster deposition system.

MM 15.68 Mon 18:00 Poster E

In detail 3D Atom Probe investigation of Tantalum capped CoFeB layers — •Patrick Stender, Houari Bouchikhaoui, and Guido Schmitz — Institut of Materials Physics, WWU, Münster, Germany

The tunnel magnetoresistance (TMR) is an important physical effect used in current technology. The TMR ratio is influenced by various parameters. Very high TMR ratios can be obtained in CoFeB/MgO based magnetic tunnel junctions. However, the TMR is strongly influenced by the capping material. Choosing Tantalum as a capping material, the TMR can be increased drastically, after a defined heat treatment. We present an atom probe study of a model MgO/ CoFeB/Ta system. In the as-prepared state, the CoFeB layer exhibits an amorphous structure Different Isochronal and isothermal annealing sequences have been carried out to investigate the structural changes and reactions. Observed diffusion and segregation processes of Boron have been identified and quantified.

MM 15.69 Mon 18:00 Poster E

A molecular dynamics study of crack/void interaction in α-Iron — •Tianxiang Liu, Sebastien Groh, and Abdolhamid Attaran — Institute for Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Lampadiusstr. 4, 09596 Freiberg, Germany

When a crack front interacts with an array of a second-phase inclusions, it bends to an angle before it moves furthers. Depending on the strength of the inclusions, the crack front either remains relatively straight or bows between inclusions and moves deeply along the easy path. The resistance to crack growth is therefore changed by the presence of inclusions.

In this paper, we are presenting a study on crack/void interaction using molecular dynamics. α-iron modeled with an EAM potential was considered. Three distributions of void were considered: (i) void positioned at varying distance normal to the crack tip, (ii) void inserted at varying distances along the crack-tip and (iii) void placed in such a way that dislocations nucleated at the crack tip reached the void when moving. The data obtained for the different configurations were compared to the ones obtained in a void free specimen.

Depending on the configuration, elastic shielding or anti-shielding was observed as a function of the temperature and strain rate. The increase in temperature would augment the shielding effect in all the configurations. The anti-shielding effect was detected in the first configuration. This effect diminished as the void was moved away from the crack tip as expected by elasticity.

MM 15.70 Mon 18:00 Poster E

$SrRuO_3/Pr_{0.7}Ca_{0.3}MnO_3$ epitaxial multilayers: A HAADF-STEM, EDX and image simulation study — •Eckhard Pippel[1], Reinald Hillebrand[1], Ionela Vrejoiu[2], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle (Saale), Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

The electrical and magnetic properties of perovskite multilayer structures strongly depend on the interface morphology between the single layers. We study the interfaces of PLD-grown epitaxial multilayer stacks of $SrRuO_3/Pr_{0.7}Ca_{0.3}MnO_3$ (SRO/PCMO) by means of probe-corrected (C_s=0) scanning transmission electron microscopy (HAADF-STEM) including energy dispersive X-ray analysis (EDX). It is possible to clearly distinguish different chemical terminations of the single layers as well as varying degrees of intermixing, if image simulations are utilized. The interfaces are evaluated by matching the intensities of the related atomic columns with simulated HAADF-STEM patterns of crystallographic super-cell models, supported by atomically resolved chemical analysis (EDX). All these techniques proved the interfaces to be affected by intermixing over two (PrO-terminated) or one (SrO-terminated) lattice planes. In practice, a series of annealing experiments of the SRO/PCMO specimens was performend to find out the temperature stability of these perovskite multilayers. The temperatures applied were between 725°C and 1200°C. In summary it is stated that already Z-dependent HAADF-STEM images offer a fairly good atomically resolved insight into intermixing phenomena.

MM 15.71 Mon 18:00 Poster E

Mechanical influences on lithium ion battery electrodes — •Tobias Kitzler[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholz-Zentrum Geesthacht, Institut für Werkstoffmechanik, Werkstoffforschung — [2]TU Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie

Lithium ion batteries have drawn major attention during the last years. One very promising attempt to get batteries with better performance is to reduce the structure size of the electrodes which leads to very high surfaces and therefore improved kinetics. Besides this, downscaling seems to be a promising way to omit crack formation due to volume change which is the most important capacity loss mechanism in lithium alloy negative electrodes. On the other hand, downscaling leads to mayor stress evolution due to volume change, which according to the thermodynamic Maxwell relations, changes the electrochemical potentials. This influence has been observed in different experiments, but was not yet quantitatively measured. Here a setup is presented which allows to quantitatively measure the influence of uniaxial strain

on the electrochemical properties of lithium ion electrodes. Therefore, dense and nanoporous Au films, synthesised by sputtering of pure Au and Au32Ag68, followed by an electrochemical dealloying process respectively, on a polyimide substrate were oscillatory strained and the corresponding change of the chemical potential recorded and analysed with respect to its impact on the kinetics of the loading and unloading processes as well as microstructural changes of the electrode itself.

MM 15.72 Mon 18:00 Poster E

Transmission electron microscopy study of defects in BiFeO3 thin films — •Hakan Deniz, Akash Bhatnagar, Eckhard Pippel, Marin Alexe, and Dietrich Hesse — Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle (Saale), Germany

A wide class of oxide materials with perovskite crystal structure has been in the focus of intense research efforts lately due to fascinating properties they posses; such as ferroelectricity, colossal magnetoresistance, superconductivity, etc. Bismuth ferrite (BiFeO3) among them is the leading contender in the research of multiferroic compounds with both ferroic order parameters well above room temperature. It is of vital importance to grow defect-free high quality thin films in order to better understand/correlate structure-property relationships of these materials. Single crystal BiFeO3 thin films grown by pulsed laser deposition on scandate oxide substrates (TbScO3, GdScO3, etc.) have been investigated in high-resolution TEM (HRTEM) and high angle annular dark field scanning TEM (HAADF-STEM). Defects having a layered structure, similar to bismuth-oxide layered perovskites, with a chemical composition different from the rest of the film have been observed. Fast Fourier transform (FFT) analysis and image processing were used to elucidate the nature of these defects. They correspond to a new unknown phase in BiFeO3 thin films. Understanding their origin will help to grow higher quality virtually defectless films. This work is supported by the FP7 project IFOX.

MM 15.73 Mon 18:00 Poster E

In situ transmission electron microscopy study of the crystallization of bits in Ag4In3Sb67Te26 — •Manuel Bornhöfft[1,2], Andreas Kaldenbach[3], Matthias Wuttig[3], and Joachim Mayer[1,2] — [1]Central Facility for Electron Microscopy, RWTH Aachen University, Aachen, Germany — [2]Ernst Ruska-Centre, Forschungszentrum Jülich, Jülich, Germany — [3]I. Physikalisches Institut (IA), RWTH Aachen University, Aachen, Germany

The understanding of crystallization kinetics of phase-change materials is mandatory to develop reliable and fast phase-change data-storage devices, which can surpass actual data-storage technologies. A topic of interest is the role of nucleation and growth in phase-change materials at different conditions.

In this work in situ-methods in a transmission electron microscope are used to observe the crystallization of round amorphous marks (bits) in a crystalline matrix of the phase-change material Ag4In3Sb67Te26. The in situ-methods employed are based on crystallization by in situ-heating and in situ-irradiation by the focused electron beam in the microscope. The bits with 0.6 μm in diameter are produced by laser irradiation of a 30 nm thick crystalline layer of the phase-change material. The phase-change layer is embedded in a 160 nm thick supporting multilayer stack. The supporting layers are amorphous and the phase-change layer is crystallized through ex situ-heating.

The results are compared with experimental observations on Ge2Sb2Te5 and give important insight in the crystallization mechanisms and the underlying thermodynamic processes.

MM 15.74 Mon 18:00 Poster E

TEM study of annealed γ-Al_2O_3-coatings for cutting tools and of γ-Al_2O_3-coated cutting tools after the use in cutting tests — •Merlin G.J. Müller[1], Joachim Mayer[1], Susanne E. Cordes[2], Kirsten Bobzin[3], Nazlim Bagcivan[3], Mara Ewering[3], and Ricardo H. Brugnara[3] — [1]Central Facility for Electron Microscopy, Aachen, Germany — [2]Laboratory for Machine Tools and Production Engineering, Aachen, Germany — [3]Surface Engineering Institute, Aachen, Germany

Among the transition aluminas, the γ-Al_2O_3-phase has a high potential for the use as hard coating in many technological applications, because it exhibits excellent properties e.g. high hot hardness and high thermal stability. It can also be deposited by means of physical vapor deposition at lower temperatures (below 700 °C) than the stable α-Al_2O_3 phase, deposited by means of chemical vapor deposition (about 1000 °C). Thus, even temperature sensitive materials can be coated and the resulting alumina layer is rather fine-grained which should lead to better mechanical properties. The phase transformation of the metastable γ-Al_2O_3-phase into the stable α-Al_2O_3-phase at high temperatures can cause cracks or even the delamination of the coating. To investigate the phase stability of γ-Al_2O_3-coatings, the structure of annealed samples and of samples after the use in cutting tests were characterized by Transmission Electron Microscopic-methods. The γ-Al_2O_3-coatings were deposited by means of Magnetron Sputter Ion Plating on cutting inserts with a (Ti,Al)N-interlayer or directly onto Si-wafers.

MM 15.75 Mon 18:00 Poster E

Ultrathin TEM lamellae for low voltage Cs-corrected STEM — •Andriy Lotnyk, David Poppitz, Ulrich Ross, Jürgen W. Gerlach, Eric Thelander, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Permoserstr. 15, 04318 Leipzig, Germany

For high-resolution aberration-corrected (Cs-corrected) low voltage scanning transmission electron microscopy (STEM) the quality of investigated TEM samples is crucial. The TEM specimens should be thinner as 10 nm. Nowadays, widely used focused ion beam (FIB) preparation techniques cannot be employed in fabrication of thin TEM samples with a thickness less than 10 nm. In the present work, we investigate the preparation of different thin film materials and interface structures for analysis in low voltage Cs-corrected STEM using FIB lift-out method followed by low energy Ar-ion polishing (less than 1 kV) in a NanoMill low energy ion mill system. Using this approach we are able to routinely prepare large area TEM lamellae with thicknesses below 10 nm. The resulting TEM specimens are suitable for low voltage STEM. We have demonstrated atomic resolution by Cs-corrected STEM at 80 kV.

MM 15.76 Mon 18:00 Poster E

Study of Solid Solution Strengthening of Nickel by transition metal solutes using Diffusion couples and Nanoindentation — •Hamad ur Rehman, Mathias Göken, and Karsten Durst — Institute of General Materials Properties, Department of Material Science, FAU erlangen-Nürnberg

Diffusion couples are often used for the determination of phase diagrams. In the present work, nanoindentation was used on diffusion couples to measure solid solution strengthening in Nickel based alloys. By combining Nanoindentation with the chemical composition, measured by EDX a very high spatial resolution is achieved in the Interdiffusion zone. It was applied to the development of Nickel based super alloys, which have more than 15 alloying elements. While some of these are gamma prime formers, others act as solid solution strengtheners for the matrix. Therefore, it is important to understand the contribution of these alloying elements on solid solution strengthening. Ni-NiX (X = Ta, W, Re, Ir and Pt) diffusion couples were used to study the influence of transition metal elements on solid solution hardening (SSH) of Nickel. The SSH was evaluated using Labusch theory. It was found that the solid solution hardening coefficient is dependent on the size of the solute elements and their atomic number. These results show that the solid solution strengthening depends on the atomic radius and the corresponding electronic structure of the solute elements. This combinatory approach allows us to determine the SSH coefficients as a function of the composition of the solid solution hardening element.

MM 15.77 Mon 18:00 Poster E

Characterizing the origin of the collapse of the channeling circle in aberration-corrected HRTEM — •Alexander Surrey[1,2], Darius Pohl[1,2], Ludwig Schultz[1,2], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany. — [2]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

Calculations of the complex electronic exit wave functions (EWFs) of model structures utilizing multi-sclice algorithms in combination with HRTEM contrast simulations reveal that the amplitudes and phases of these reconstructed EWFs lead to a collapse of the channeling circle when "real" samples are investigated under realistic microscopy conditions. As a consequence, the reconstruction of the 3D structure of the samples by means of the acquisition of focal series of HRTEM images becomes impossible. A detailed analysis shows that this collapse is caused by the accumulation of contributions from (i) the modulation transfer function of the camera, (ii) slight misorientations of the sample, (iii) inelastic absorptions, (iv) amorphous overcoats or substrates, and (v) equilibrium as well as athermal phononic excitations. The collapse becomes most easily evident from a significant lack in the phase signal derived from the EWFs. Whereas the phase shift asso-

ciated with moving along the channeling circle in the Gaussian plane should successively grow to the full range of 2π, the phases determined from the EWFs frequently amount to only fractions of π. This limited phase range is confirmed by the EWF recontructions determined from experimental through focus series of thin Au nanostructures acquired with an aberration-corrected FEI Titan^3 80-300 microscope.

MM 15.78 Mon 18:00 Poster E

Investigation of metal droplets on dilute Bi-containing III-V semiconductors — •Eduard Sterzer, Nikolai Knaub, Peter Ludewig, Wolfgang Stolz, and Kerstin Volz — Material Sciences Center and Department of Physics, Philipps-University Marburg, Germany

Dilute bismuth (Bi)-containing III-V semiconductors are interesting from the application point of view, as Bi increases the spin-orbit splitting in conventional III-V semiconductors. The epitaxial growth of these materials is a big challenge due to the formation of metal droplets on the surface. In order to grow droplet free layers a better understanding of the formation process of these droplets is necessary. In this study the surface morphologies of Ga(BiAs)/GaAs structures grown by metal organic vapor phase epitaxy are investigated by scanning electron microscope and atomic force microscope (AFM). Energy dispersive X-ray spectroscopy was used to determine the composition of the droplets. Furthermore the crystal structure was analysed by transmission electron microscopy (TEM). In dependence on the V/III ratio as well as the growth temperature we observe pure Bi- droplets or mixed Ga-Bi droplets. The investigation of the morphology using AFM gives an indication of the droplets moving on the surface during growth. The crystal structure around the droplets and the structure of the droplets itself was investigated with transmission electron diffraction as well as high resolution TEM and will be correlated to the growth conditions.

MM 15.79 Mon 18:00 Poster E

TEM dark-field characterization of anti phase domain boundaries in GaAs on Ge — •Lukas Nattermann, Tatjana Wegele, and Kerstin Volz — Structure and Technology Research Laboratory, Materials Science Center and Faculty of Physics Philipps-Universität Marburg, Germany

The use of GaAs on Ge in multijunction solar cells requires a high crystal quality and a defect-free GaAs/Ge interface. For the characterization of the GaAs-layer and the GaAs on Ge boundary we used transmission electron microscopy (TEM). Additionally we compared GaAs on Ge to GaP on Si with respect to the anti phase domain (APDs) boundaries. In order to investigate the influence of such growth-parameters as temperature and the atom types in the monolayer between GaAs and Ge, three MOVPE (metal organic vapour phase epitaxy)-grown GaAs/Ge - samples were examined by using the TEM dark-field (DF)-technique. To verify APDs with the help of contrast reversal we used the (002)- and (00-2)-DF-reflections. We study specimens in three different zone axes, [001], [110] and [1-10], to get an idea of the three dimensional shape of the anti phase domains. We can show the difference of the shape of APDs in GaAs on Ge and GaP on Si and the influence of the insufficient pretreatment of the Ge-substrate. Moreover we determine the directions of the propagation planes of the APD-boundaries and analyze the size of the APDs.

MM 15.80 Mon 18:00 Poster E

Quantitative study of electron-radiation damage by in situ EFTEM investigations of the phase transformation from $CaCO_3$ to CaO at 80 kV, 40 kV and 20 kV — •Werner Schweigert[1], Ute Golla-Schindler[1], Gerd Benner[2], and Ute Kaiser[1] — [1]Group of Electron Microscopy of Materials Science, Central Facility of Electron Microscopy, 89081 Ulm, Germany — [2]Carl Zeiss NTS GmbH, Application TEM / Materials Analysis, 73447 Oberkochen Germany

The TEM investigation showed that under electron irradiation a phase transformation from $CaCO_3$ to CaO occur. (This is the transformation route for CaO (quicklime) production out of calcite, taking place at elevated temperatures of 900 °C.) The phase transformation is accompanied by a strong volume loss of the particles. We developed a method for measuring quantitatively the volume loss in dependence of the particle thickness and the accelerating voltage of the microscope. The determination of the volume is divided in two parts. Our method for segmenting the image into vacuum and particle is an edge detection process based on the canny algorithm. The thickness can be measured with the log-ratio method. The TEM investigations were performed on the SALVE (Sub-Angström Low-Voltage Electron) prototype microscope equipped with an image-side Cs-corrector, a field emission gun, a monochromator and a corrected in-column OMEGA energy filter. TEM studies were performed at 20, 40, 80 kV. We found that the volume-loss is dose-rate dependent and increases with lower voltages; the contrast however is increasing.

MM 15.81 Mon 18:00 Poster E

Electron irradiation effects on QDs in TEM and SEM — •Thomas Kister, Ute Golla-Schindler, and Ute Kaiser — Group of Electron Microscopy of Materials Science, Central Facility of Electron Microscopy, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Monodisperse CdSe/CdZnS QDs, which are capped with trioctylphosphine oxide (TOPO), have a high fluorescence quantum yield. They are for example supposed to be used in the near future as marker for biological matter in medicine. Up to now the chemical and structural constitution on the atomic level is not well known. Unfortunately, in the initial investigation it was indicated that QDs are losing their fluorescence abilities dramatically by electron irradiation already at low dose rates. Therefore we started systematic studies of radiation damage dependence on dose, dose rate and accelerating voltage. For the experiments the TOPO-capped QDs, which are suspended in hexane, are deposited on carbon and silicon oxide filmed TEM-grids. The fluorescence of the QDs is measured before and after electron irradiation with an optical microscope (Zeiss Axioscope 2 mot plus). A Philips CM20 TEM and a Zeiss NVision 40 SEM are used for the electron irradiation investigations. Through these experiments we hope to get a better understanding of the interaction and irradiation mechanisms taking place during the electron microscopy studies.

MM 15.82 Mon 18:00 Poster E

Reduction of Radiation Damage in Ultrathin MoS_2 — •Mona Sedighi, Simon Kurasch, Gerardo Algara-Siller, and Ute Kaiser — Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm, Germany

Previous high-resolution transmission electron microscopy (HRTEM) experiments [1] on free-standing single layer MoS_2 reported that, at an acceleration voltage of 80 kV, the material suffers from knock-on damage via removal of sulfur atoms from the beam exit surface. Similar to earlier work on graphene [2] it is possible to extract the sputtering cross section from atomically resolved HRTEM time series.

Here we report that, covering the electron exit surface of the free-standing single-layer MoS_2 by single-layer graphene serves to minimize the radiation damage. Moreover, comparing the response to high electron irradiation of free-standing MoS_2 to top-side covered and bottom-side covered MoS_2 allows separating the effect of ionization and chemical damage from the total damage that initially was attributed only to sputtering.

[1] H. Komsa et al., Phys. Rev. Lett 109, 035503 (2012)
[2] J. Meyer et al., Phys. Rev. Lett 108, 196102 (2012)

MM 15.83 Mon 18:00 Poster E

Voltage contrast in SEM for revealing charge transport through metallic nanowire transparent electrodes — •Stefanie Spallek[1], Johannes Krantz[2], Peter Kubis[2], Johannes Holzmair[3], Silke Christiansen[3], Christoph J. Brabec[2], Benjamin Butz[1], and Erdmann Spiecker[1] — [1]CENEM, University of Erlangen-Nürnberg — [2]I-MEET, University of Erlangen-Nürnberg — [3]MPI for the Science of Light, Erlangen

Metallic nanowire (NW) transparent electrodes are of special interest in research and economy due to their cheap and scalable printing production process, their high optical and electrical quality and their application possibility to flexible devices. However charge transport through metallic NW networks is not yet well understood. Here, we report on a voltage contrast dependent scanning electron microscopy (VC-SEM) study of metallic NW electrodes near the electrical percolation threshold. As the properties of NW junctions within the network directly lead to the properties of the whole electrode, e.g. sheet resistance, they are of special interest in this study. NW junctions are insolating until the voltage threshold is reached, whose value presumably is depending on the insulating layer of process residues. By exceeding the voltage threshold the NW junction seems not to balance the amount of charge carriers on both sides, though. Therefore, the contrast mechanism of VC-SEM of metallic NWs was studied to quantify the voltage difference. In addition we show a VC-SEM study of metallic NW electrodes ready for application with which a potential drop of 0 to 8 Volts over a distance of several microns was observed.

MM 15.84 Mon 18:00 Poster E

Freely suspended membranes from epitaxial graphene on silicon carbide — •Christian Dolle[1], Benjamin Butz[1], Daniel Waldmann[2], Heiko Weber[2], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg

We present a route to produce freely suspended graphene membranes by thermal decomposition of SiC(0001) at 1760° C under reduced inert gas atmosphere yielding a mean of 1.2-1.5 layers of high crystalline-quality graphene. Laser-assisted electro-chemical removal of the SiC substrate in KOH at lithographically predefined areas allows us to tailor the number and shapes of the membranes with sizes up to at least 500 μm^2. We carried out a thorough characterization of the freely-suspended membranes employing Raman spectroscopy, SEM, low-kV-STEM and plan-view TEM. The powerful tool of abberation-corrected TEM can resolve the spatial distribution of one up to four graphene layers on the membranes and contrast variation in dark-field imaging allows a straightforward and facile assignment of the number of layers. One of the great benefits of the preparation procedure is the high cleanliness of the samples, allowing high resolution imaging even without the need of precedent heat treatment although the membranes withstand in-situ thermal exposure up to 1000° C in vacuo without mentionable damage.

MM 15.85 Mon 18:00 Poster E

Structural Analysis of Nickel Doped Cobalt Ferrite Nano Particles Prepared by Coprecipitation Method — Mahbube Houshyar[1], •Ali Alidoust[1], Zohre Askari[1], Zahra Jafari[1], and Fateme Zebhi[2] — [1]Shahid beheshti,Tehran,Iran — [2]Semnan,Semnan,Iran

in this research nano particles of cobalt ferrite ,nickel cobalt ferrite and nickel ferrite have been synthesized using coprecipitation method. size of the every particles have been obtained by XRD and analyses of UV , FTIR , SEM , DLS and VSM have been done on the nano powders and the size , light absorption , dynamic light scattering , coercivity , retentivity and saturation magnetization of the particles have been compared.

MM 15.86 Mon 18:00 Poster E

In-situ and ex-situ ACOM-STEM analysis of the direction dependent deformation behavior of nanotwinned copper — •Aaron Kobler[1,2], M. Funk[3], C. Eberl[3], A. Hodge[4], Horst Hahn[1,2], and Christian Kübel[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, 76021 Karlsruhe, Germany — [2]Technische Universität Darmstadt (TUD), KIT-TUD Joint Research Laboratory Nanomaterials, 64287 Darmstadt, Germany — [3]Karlsruhe Institute of Technology (KIT), Institute of Applied Materials, 76021 Karlsruhe, Germany — [4]University of Southern California, Department of Aerospace and Mechanical Engineering, Los Angeles, California 90089-1453, USA

Nanotwinned (nt) metals as a class of nanostructured materials have been receiving considerable attention as they combine the high strength of nanocrystalline (nc) metals with a higher ductility and higher thermal stability compared to the corresponding nc metals. Face-centered cubic metals with low stacking fault energy like Cu have the tendency to develop this kind of nt structure. Although twin boundaries are thermodynamically more stable than random grain boundaries, they can become unstable under mechanical load. The deformation behavior of magnetron sputtered nt Cu was studied using ex-situ and in-situ TEM techniques combining classical BF/DF-TEM analysis with the recently developed automated crystal orientation mapping (ACOM-TEM). Two straining directions were tested in-situ, one parallel to the twin plane and one perpendicular to it and compared to the ex-situ deformation parallel to the twin plane on ~20μm thick bulk samples. The straining experiments show a significant difference between bulk and thin film deformation as well as a strong orientation dependence in the thin film.