MM 26: Poster Session

Time: Tuesday 14:45–16:30 Location: Poster C

MM 26.1 Tue 14:45 Poster C

Ultra-fast diffusion paths in nickel after ECAP — •Gerrit Reglitz, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

The concept of so called "non-equilibrium" grain boundaries describes a specific (highly defected) type of grain boundaries in materials, which are produced by severe plastic deformation like ECAP (equal channel angular pressing) or high-pressure torsion. These specific grain boundaries are supposed to have a high density of extrinsic (excess) grain boundary dislocations, and, thus, higher excess grain boundary energy, larger free volume and enhanced diffusivity. To investigate the different types of grain boundaries in Ni after severe plastic deformation by ECAP the self-diffusion experiments were carried out by using the ^{63}Ni isotope in combination with a parallel sectioning technique. The results of these investigations highlight the existence of different types of grain boundaries in this material with completely unequal diffusion characteristics. The kinetic properties are dramatically affected by a preliminary heat treatment. The concept of the "non-equilibrium" grain boundaries in severely deformed materials is critically discussed on the basis of the present data. Support by DFG is gratefully acknowledged.

MM 26.2 Tue 14:45 Poster C

Individual precipitates in Al alloys probed by the Bonn Positron Microprobe — Osman Balarisi[1], Patrick Eich[1], Matz Haaks[1], Sven-Martin Hühne[2], •Benedikt Klobes[1], Björn Korff[1], Werner Mader[2], Karl Maier[1], Reinhard Sottong[1], and Torsten Staab[3] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn — [2]Institut für Anorganische Chemie , Römerstraße 164, 53117 Bonn — [3]Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg

Positron annihilation spectroscopy (PAS) is a unique tool for the charaterization of open-volume defects such as vacancies. Therefore, age hardenable Al alloys, whose decomposition is mainly driven by the vacancy mechanism of diffusion, are often charaterized by PAS techniques. Nevertheless, probing the defect state of individual precipitates grown in Al alloys requires a focused positron beam and has not been carried out up to now. In this respect we present the first investigations of the defect state of individual precipitates utilizing the Bonn Positron Microprobe (BPM). Furthermore, the analysis of the experimental data has to be facilitated by theoretical calculations of the observables of positron annihilation spectroscopy.

MM 26.3 Tue 14:45 Poster C

Comperative study of point defects in *n*-type TCO materials — •Péter Ágoston[1], Paul Erhart[2], Andreas Klein[1], Risto M. Nieminen[3], Martti J. Puska[3], and Karsten Albe[1] — [1]Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, 64287 Darmstadt — [2]Lawrence Livermore National Laboratory, L-367, Livermore, CA 94550, USA — [3]Department of Applied Physics, Helsinki University of Technology, FIN-02015 TKK, Finland

The performance of transparent conducting oxides (TCO) is strongly interrelated with their point defect thermodynamics and kinetics. In this contribution we present first-principles calculations on the point defects and their migration in typical *n*-type TCO materials. We focus on the TCO materials In_2O_3, SnO_2, ZnO, CdO and Ga_2O_3. We have conducted total energy calculations within the framework of density-functional theory on a semi-local level and in conjunction with the nudged elastic band method to obtain the formation and migration energies for all relevant defects in several charge states. The defect formation energies are corrected using the hybrid functional DFT methodology and are therefore not affected by the DFT band gap error. Within this band gap error free description we present the general trends of the point defect thermodynamics and kinetics in these materials and also point out important differences.

MM 26.4 Tue 14:45 Poster C

Atomic-Scale Modeling of Diffusion-Driven Microstructure Evolution in Irradiated Metals — •Erik Bitzek[1,2], Sanket Sarkar[3], William T. Cox[3], Thomas Lenosky[2], Yunzhi Wang[3], and Ju Li[2] — [1]Lehrstuhl Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg — [2]Department of Materials Science and Engineering, Ohio State University, Columbus, OH, USA — [3]Department of Materials Science and Engineering, School of Engineering and Applied Science, University of Pennsylvania, Philadelphia, PA, USA

Diffusion of vacancies and impurities plays an important role in irradiated materials. The elementary diffusion processes are readily studied at the atomic scale and the results can be used to compile event catalogs needed by kinetic-Monte-Carlo (kMC) simulations of diffusion. However, the interplay between diffusion and changes in the microstructure remains less well understood, as it involves not only random motion of vacancies in stress gradients but also the concerted motion of atoms, e.g. during dislocation nucleation or glide. The different time scales involved in these processes pose a general challenge to modeling approaches.

Here we present a novel computational method, termed diffusive molecular dynamics (DMD), which allows for the study of diffusion driven evolution of complex microstructures at the atomic scale. The utility of DMD to investigate processes related to irradiation damage is demonstrated by studies on void formation and growth and the creation of stacking fault tetrahedra (SFT).

MM 26.5 Tue 14:45 Poster C

Introducing variable barrier heights in Kinetic Monte-Carlo simulations: A study of order-order transitions in $L1_2$ ordered Ni_3Al based on first-principles calculations — •Martin Leitner[1], Doris Vogtenhuber[2], Wolfgang Pfeiler[1], and Wolfgang Püschl[1] — [1]University of Vienna, Faculty of Physics, Department Dynamics of Condensed Systems — [2]University of Vienna, Faculty of Physics, Department of Computational Materials Science

Kinetic Monte-Carlo (KMC) simulation is a valuable tool when it comes to studying atom jump behavior in detail, for instance the kinetics of the long-range ordered state in intermetallics which is a precondition for a lot of favorable material properties. We introduce an improved KMC algorithm with variable saddle point heights depending on atom environment. In transition state theory the barrier height is the energy difference between the initial equilibrium state and a saddle point state which was mostly set constant in traditional treatments. In contrast, taking $L1_2$ ordered Ni_3Al as a model system, an explicit calculation of the saddle point height is proposed and demonstrated. It is seen that the 4-atom window through which the jumping atom has to pass is decisive. We calculated *ab initio* a complete set of jump energy profiles for all possible jump types and window occupations. In KMC simulations we tested the influence of this explicit calculation and compared it to the old paradigm of constant saddle point heights. It turned out that individually computed saddle point energies make a considerable difference in jump statistics and overall kinetics.

MM 26.6 Tue 14:45 Poster C

Investigation of Li dynamics in gas-phase synthesized amorphous oxides by NMR and impedance spectroscopy — •Viktor Epp, Christian Brünig, Martin Wilkening, Michael Binnewies, and Paul Heitjans — Leibniz Universität Hannover, D-30167 Hannover

Currently, great effort is put into finding novel ion conductors that meet the requirements of modern energy storage systems. The characterization of their transport properties with complementary methods plays a crucial role in this research area. Here, metastable, highly non-stoichiometric oxides containing Al, Li and Si were studied by impedance spectroscopy (IS) and, complementarily, by various ^{7}Li NMR techniques which are capable to probe Li dynamics on different time and length scales [1, 2]. The samples, which are X-ray amorphous, were synthesized via a gas-phase reaction [3] from $AlCl_3$, LiCl and $SiCl_4$. The applied NMR techniques included the analysis of ^{7}Li NMR spin-alignment echoes, line shapes as well as spin-lattice relaxation (SLR) rates $T_{1\rho}^{-1}$ in the rotating frame of reference. When probed on the same time scale, good agreement is found between the activation energies obtained from IS and SLR NMR. Altogether, the Li diffusivity in the investigated oxide turned out to be rather slow.

[1] M. Wilkening, V. Epp, A. Feldhoff, P. Heitjans, J. Phys. Chem. C 112 (2008) 9291.
[2] M. Wilkening, P. Heitjans, Phys. Rev. B 77 (2008) 024311.
[3] T. Giesenberg, S. Hein, M. Binnewies, G. Kickelbick, Angew.

Chem. Int. Ed. 43 (2004) 5697.

MM 26.7 Tue 14:45 Poster C

Interplay between structural disorder and magnetic susceptibility in FeSi — •Tommy Reimann, Dirk Menzel, Dirk Schulze Grachtrup, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

The narrow gap semiconductor FeSi has been of high experimental and theoretical interest for over 60 years, mostly due to its unusual magnetic behavior. To clarify the reasons for the Curie-Weiss-like reincreasing of the magnetic susceptibility at low temperatures, we performed transport and susceptibility measurements on different FeSi single crystals grown via the tri-arc Czochralski method. A part of the FeSi samples, which were grown with slightly different stoichiometry close to 1:1 were annealed at 1000°C for 3 months. The susceptibility measurements reveal a reduction of the Curie-constant due to the annealing process. In addition, samples with iron excess show a smaller residual susceptibility compared to crystals with iron deficit. This fact cannot be explained by the often claimed assumption that uncompensated iron carries the magnetic moment. The observed appearance of variable range hopping conductivity in combination with a negative magnetoresistivity suggests that Anderson-localized electrons caused by structural disorder induce the low temperature Curie-Weiss-like behavior.

MM 26.8 Tue 14:45 Poster C

First-principles study of the structural and electronic properties of CuO as grown on SrTiO$_3$ — Cesare Franchini[1], Xing-Qiu Chen[2], and •Raimund Podloucky[3] — [1]Faculty of Physics, Univ. of Vienna, Vienna, Austria — [2]Shenyang National Laboratory for Materials Science, Shenyang, China — [3]Faculty of Chemistry, Univ. of Vienna, Vienna, Austria

Very recently, a tetragonal phase of antiferromagnetic CuO was synthesized by growing it epitaxially on a SrTiO$_3$ substrate. In a previous paper [1] we modeled the tetragonal CuO phase by a freestanding block of material simulating the epitaxial effect by fixing the lateral lattice parameters and relaxing the c/a ratio. Applying a hybrid-functional density-functional-theory approach two tetragonal phases were identified whereby the phase with $c/a = 1.38$ perfectly matches the basic experimental structural parameters. However, its electronic structure shows some significant deviations from the experimental valence band spectra. In the present study the effect of the substrate is explicitely taken into account by placing CuO layers with different thicknesses on top of a SrTiO$_3$(100) substrate. Several substrate terminations as well as structural relaxations are considered in order to search for the most stable atomic arrangement. The resulting ground state electronic and structural properties as a function of the thickness of the CuO layer are discussed. For the actual calculations the Vienna Ab initio Simulation Package (VASP) in combination with its hybrid functional features is applied.

[1] X.-Q. Chen et al., Phys. Rev. B **80**, 094527 (2009).

MM 26.9 Tue 14:45 Poster C

Stable and unique solutions for the OEP equation in the LCAO formalism — •julio juan fernandez[1], Christian Kollmar[2], and Michael Filatov[1] — [1]Institute for Advanced Materials, Groningen 9747 AG The Netherlands — [2]Institut fur Physicalische und Theoretische Chemie, Bonn D53115 Germany

The treatment of orbital dependent functionals in Density Functional Theory (DFT) requires the use of the Optimized Effective Potential (OEP) technique for obtaining the local multiplicative potential. Using the exchange only (xOEP) functional this formalism leads to an equation that, in real space, possesses a unique and well defined solution for atoms and molecules. In a basis set (LCAO) scheme the method leads to a non unique solution of the equation due to the singularity of the matrix representation of the linear response operator. In this work we demonstrate that a good solution to this problem is to use an incomplete Cholesky decomposition of the linear response matrix. With the use of this technique numerically stable and unique solutions of the xOEP equations in the LCAO representation are obtained provided that the orbital basis set satisfies the condition of linear dependence of the products of occupied and virtual Kohn_sham orbitals. It is demonstrated that the obtained LCAO-xOEP solutions are independent on the criterion used to discriminate linearly dependent from linearly independent (ia) products.

The LCAO-xOEP solutions for atoms and molecules are obtained with the use of standard basis sets. The LCAO-xOEP energies are in excellent agreement with the numeric real space xOEP energies.

MM 26.10 Tue 14:45 Poster C

Thermomechanical properties of mullite up to 1673 K: single crystal vs. ceramics — •Thomas Friedrich Krenzel[1], Jürgen Schreuer[1], and Hartmut Schneider[2] — [1]Ruhr University Bochum, Institute of Geology, Mineralogy and Geophysics, Bochum, Germany — [2]University of Cologne, Institute of Crystallography, Köln, Germany

The poster by Adel Benlagra originally scheduled for MM 26.10 has been moved to TT 27.21.

Ceramics with mullite composition are well known and appreciated for their favourable properties like high thermal stability, low thermal expansion and conductivity or high creep resistance. They are extensively used as high temperature application materials e.g. like kiln furnitures, catalytic convertors, coatings or engineering ceramics.

Schreuer et al. [1] recently studied the mechanical properties of single crystals up to 1673 K and found an anomaly in the temperature evolution of the strains parallel to principle axes and furthermore a strong deviation from linearity of observed shear stiffnesses compared to calculated ones, both above about 1273 K. They proposed a glass-like transition at this temperature. Another research group interpreted similar or stepwise anomalies of different properties at same temperatures as a phase transition [2; 3].

Since this anomaly is not yet fully clarified the goal of this work is to bring up new aspects by a comparison of thermal expansion and elastic properties of mullite ceramics, which were prepared in different ways, with new single crystal data of higher resolution up to 1673 K. The measurements of thermal expansion and elastic properties were done with the help of dilatometry and resonant ultrasound spectroscopy, respectively.

MM 26.11 Tue 14:45 Poster C

Bestimmung von Fermi-Flächen in dünnen Schichten mittels 2D-ACAR — •Hubert Ceeh, Christoph Hugenschmidt und Peter Böni — Pysik Departement E21, Technische Universität München

Wird ein Positron in einen Festkörper implantiert, thermaliert es innerhalb weniger Picosekunden. Daher ist der Schwerpunktsimpuls des Systems aus Elektron und Positron bei der Annihilation praktisch ausschließlich durch den Impuls des Elektrons bestimmt. Die transversale Impulskomponente führt dabei zu einem von 180 Grad abweichenden Winkel zwischen den Annihilationsquanten. Aus der Messung dieser Winkelkorrelation (ACAR: Angular Correlation of Annihilation Radiation) mittels zweier Anger-Kameras können somit Rückschlüsse auf die Impulsverteilung de Elektronen gezogen werden. Im Gegensatz zu Messungen der Fermifläche unter Ausnutzung des De-Haas-van-Alphen-Effekts sind Messungen mit der ACAR-Methode bei Temperaturen von bis zu 400K möglich. Des Weiteren ist man nicht auf ein starkes Magnetfeld angewiesen, was das Studium der elektronischen Struktur beispielsweise von Supraleitern erlaubt. An der hochintensiven Positronenquelle NEPOMUC wird derzeit ein ACAR-Spektrometer realisiert, um mit mono-energetischen Positronen bei erheblich verkürzter Messzeit, temperaturabhängig die elektronische Struktur in dünnen Schichten untersuchen zu können.

MM 26.12 Tue 14:45 Poster C

Relaxation of Volume and Enthalpy of Bulk Metallic Glasses — •Jonas Bünz, Joachim Bokeloh, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Although the relaxation of glasses is a phenomenon that is known for centuries and that is actually at the very foundations of the unique applicability of glasses in general - the controlled modification of properties without changes of the chemical composition - the physics behind the relaxation and aging processes that occur in glasses after initial quenching are far from being understood. In fact, it is basically still unclear whether the relaxation of the excess free volume and the relaxation of the excess enthalpy are identical processes that are governed by only one underlying mechanism. Measuring the kinetics of these properties with different methods like differential scanning calorimetry, microcalorimetry, dilatometry and the buoyancy method allow covering a broad range of temperatures and materials and offer the possibility to experimentally access the isothermal relaxation characteristics of the volume and the enthalpy directly on time scales that range from several hours to weeks. The results were evaluated in the framework of the free volume theory.

MM 26.13 Tue 14:45 Poster C

The influence of d- and f-states on structure formation - amorphous alloys containing Rare Earths as model systems — •Martin Stiehler, Michael Pleul, and Peter Häussler — Chemnitz University of Technology, 09126 Chemnitz, Germany

Amorphous phases as precursors of the crystalline state are interesting for investigating fundamental structure forming processes and the related evolution of electronic transport. During the last years we were able to show that many different classes of alloys organize themselves under the influence of a resonance interaction between the global subsystems of the electrons and the static structure. Especially for binary Al-TM alloys (TM: the transition metals of the 4th period Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu) we reported recently on an electronic influence on phase stability driven by hybridization effects between the Al-p- and the TM-d-states, showing an interesting systematics depending on the number of unoccupied TM-d-states reflected in different properties. Currently we are about to extend the investigations to systems with transition metals of the 5th and 6th period. Embedded in this class of elements are the so-called Rare Earth metals (Sc, Y, La, and the Lanthanoids). These elements exhibit very similar chemical properties although some of them (the Lanthanoids) contain f-electrons. This provides the possibility of studying the influence of magnetic influences, provided by the localized f-states, on structure formation. In this contribution we report on preliminary results concerning the static structure, the electrical resistivity and the Hall effect of the binary systems Al-Y and Al-Ce.

MM 26.14 Tue 14:45 Poster C

Molecular dynamics simulation of Ni/NiAl interfaces — •Stephen Hocker[1], Siegfried Schmauder[1], and Priyank Kumar[2] — [1]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre, Universität Stuttgart, Stuttgart — [2]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

Molecular dynamics simulations are used to study the brittle/ductile interface Ni/B2-NiAl under mechanical loading. Uniaxial tensile tests perpendicular to the interface are performed. It is shown that interfaces have influence on strain induced material failure by nucleation of defects. Crack propagation in the (001) interface is investigated by applying load via fixed displacement boundary conditions. Determined crack velocities in the interface turned out to be clearly above the crack velocities in each of the respective materials.

MM 26.15 Tue 14:45 Poster C

First-principles study of superhard SiN_x/TiN nanocomposites — •Pawel Rodziewicz and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien ICMM and Computer-Chemie-Centrum CCC, Universität Erlangen–Nürnberg

Nanocomposite materials based on TiN nanocrystalites embedded in an amorphous silicon nitride matrix with thickness of only a few atomic layers and composition close to Si_3N_4 show a superhardness similar to that of diamond. To elucidate the chemical origin of the material hardness and the exceptional strength of the SiN_x/TiN interfaces we have used DFT calculations in combination with Car-Parrinello molecular dynamics (CPMD) simulations to create and to investigate model SiN_x/TiN interface structures. As the first step we studied the initial stages of SiN_x layer formation on TiN(001) by adding successively silicon and nitrogen atoms to the TiN surface to form up to two monolayer thick SiN_x films with different composition. For a selected set of configurations, chosen on the basis of thermodynamic stability, we then applied a stepwise procedure based on heating, quenching and final geometry optimization to search for stable and energetically favorable amorphous structures of SiN_x films and stacks of SiN_x/TiN multilayers. The relative stability of the different model interface structures is analyzed in terms of Ti, Si and N coordination numbers, and the mechanical strength of the interfaces is assessed by the calculation of stress–strain curves to determine the ideal decohesion strength.

MM 26.16 Tue 14:45 Poster C

Tailoring Model Surfaces and Wettability Measurement for a Fundamental Understanding of Hot-dip Galvanizing — •Takashi Kawano[1,2] and Frank U Renner[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Steel Research Laboratory, JFE Steel Corporation, Japan

Hot-dip galvanizing is the process used widely for automotive steel sheets. The wettability of molten Zn with steel substrate is an important issue in the process. Especially, problems can be caused by substances such as Al, Si and/or Mn oxides formed on a substrate surface during the process. Many studies have been done to correlate the wettability and sample composition and/or process conditions related to the practical steel materials or process procedure.

However, the affect of the oxides on the wetting kinetics has not been well explained, because the surfaces of such steel substrates are generally too complicated to understand the fundamental wetting mechanisms.

Our work was started with preparing simple model surfaces so that fundamental wetting kinetics on well defined substrates can be studied with the sessile drop method at high temperatures. Our model surfaces were well defined oxide islands prepared by physical vapor deposition using different masks on flat Fe substrates.

In this report, preliminary data which shows a relation between initial contact angle and Al oxide coverage will be introduced. Comparing among various kinds of oxide species and modeling of the wetting kinetics will be future work.

MM 26.17 Tue 14:45 Poster C

Theoretical investigation of the adsorption of SPS and MPS at the Cl-covered Cu(100) surface — •W. Reckien[1], N.T.M. Hai[2], A. Fluegel[3], W. M. Hahn[3], A. Wagner[3], D. Mayer[3], P. Broekmann[2,3], and T. Bredow[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Department of Chemistry and Biochemistry, University of Bern, Switzerland — [3]BASF-SE, Electronic Materials, Ludwigshafen, Germany

Copper electrodeposition has attracted considerable attention over the last two decades due to its application in the state-of-the-art fabrication of integrated logic and memory devices. A detailed understanding of the synergistic and antagonistic interaction between so-called accelerator, suppressor and leveller molecules among themselfes and with the chlorine covered copper surface is still lacking.

We present the results of a first principles study of the interaction of the accelerator molecule SPS (bis-sodiumsulfopropyl-disulfide) and the corresponding MPS (mercaptopropylsulfonic acid) monomer with the Cu(100)/Cl system. We discuss different adsorption situations on the pure Cu(100) surface, on a compact c(2 x 2)-Cl adlayer and the influence of chlorine defects in the adlayer. Since the consideration of the electrolyte is crucial for an accurate description of the process, we present new models for the adsorption of SPS and MPS in the presence of a water electrolyte.

MM 26.18 Tue 14:45 Poster C

Ab-initio investigation of the interface structure of TiO_2 grown on Al_2O_3 — •Maxim Popov[1,2], Jürgen Spitaler[1,2], Claudia Walter[2], and Claudia Ambrosch-Draxl[2] — [1]Materials Center Leoben Forschung G.m.b.H, Rosegger-str. 12, 8700 Leoben, Austria — [2]Montanuniversität Leoben, Franz-Josef-Str. 18, 8700 Leoben, Austria

Oxide based layered structures are increasingly exploited for hard coatings. As a model system we study the interface between a TiO_2 thin film grown on an Al_2O_3 (0 0 0 1) substrate by sputter deposition. X-ray diffraction analysis of the sample reveals that TiO_2 grows in the rutile structure with the (1 0 0) plane parallel to the substrate. We use ab-initio calculations based on density-functional theory (DFT) combined with elasticity considerations to determine the local atomic arrangement at the interface region. Since the two materials forming the interface exhibit a rather large lattice mismatch, we first calculate the full elastic constant tensors for bulk Al_2O_3 and TiO_2. Then the interface between Al_2O_3 and TiO_2 is constructed by connecting the two surfaces in such a way that the stresses on both sides are balanced. In a next step the geometry of the complete interface is further relaxed within DFT. We present the optimized interface structure for three interfaces differing in the termination of the substrate or overlayer,respectively.

MM 26.19 Tue 14:45 Poster C

Ordering and site occupancy of ternary elements in Fe_3Al — •Thomas Rademacher[1], Thomas Kresse[1], Johannes Deges[2], Talaat Al-Kassab[3], Georg Frommeyer[2], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]MPI für Eisenforschung GmbH, Max-Planck-Straße 1,40237 Düsseldorf, Germany — [3]King Abdullah University of Science & Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia

$D0_3$-ordered Fe_3Al exhibits a number of advantageous properties, such as high-temperature strength, corrosion resistance and low cost. However, the mechanical properties (e.g. low ductility) and high-temperature stability needs to be optimized for technical use which can be performed by the addition of ternary elements. To understand their influence on these properties, the site occupancy needs to be determined.

In this study this is investigated for the ternary elements 4at.%V, 5at.%Cr, 5at.%Mn and 4at.%Ti by means of Atom Probe Tomography (APT). A special analysis algorithm allows resolving the atom layers for different measurement directions which enables determining site preferences. By comparing these APT-measurements with APT-simulations for different site occupancies and orderings, measurement artefacts can be extracted and an enhanced analysis can be performed.

MM 26.20 Tue 14:45 Poster C

X-ray diffraction studies on diamond cobalt composites — ●Andre Steffen[1], Christian Kronholz[2], Michael Paulus[1], Christoph J. Sahle[1], Manuel Ferreira[2], Wolfgang Tillmann[2], and Metin Tolan[1] — [1]TU Dortmund, Experimentelle Physik 1 / DELTA — [2]TU Dortmund, Lehrstuhl für Werkstofftechnologie

Diamond grinding tools have widely established its usage in machining and cutting of natural stone and concrete. The interface area between diamonds and cobalt in diamond cobalt composites is of essential relevance for the grinding process and has been investigated by X-ray diffraction (XRD) studies. It could be shown that graphite is formed during the manufacturing process and that graphite is the main constituent of the diamond cobalt interface area. No strong (chemical) bonding in the form of cobalt carbide could be detected. By in situ and ex situ studies on ultra fine cobalt powders the thermal induced phase transformation between face centered cubic and hexagonal closed package phase of cobalt at T=421 °C has been investigated. At T=620 °C cobalt occures only in the fcc phase while both phases exist at room temperature (RT). The phase transformation, fcc to hcp during cooling from T>421 °C to RT, strongly depends on the cooling gradient. Furthermore it could be shown that the phase transformation, fcc to hcp, can be additionally induced by pressure. High pressure (P=550 MPa) leads to a high volume fraction of hcp phase (about 95 %).

MM 26.21 Tue 14:45 Poster C

Anisotropic mechanical behavior of the ultrafine grained TiFe eutectic system — Antje Schlieter, ●Uta Kühn, and Jürgen Eckert — Helmholtzstrasse 20, IFW Dresden, 01171

The effect of temperature gradient and growth rate of an eutectic TiFe alloy have been examined. Samples have been arc melted ingots, cold crucible and tilt cast rods and rods cast by Bridgeman technique. The material exhibit different nanoscaled/ultrafine grained (ns/ufg) eutectic structure (β-Ti(Fe) solid solution (ss) + TiFe). Different cooling conditions lead to the evolution of ufg eutectic colonies with different orientation versus elongated lamella colonies with preferred orientation. Consequently, isotropic versus anisotropic mechanical properties were obtained. The alloys exhibit compressive strengths between 2200 - 2700 MPa and plasticity in the range of 7 to 19 % in compression.

MM 26.22 Tue 14:45 Poster C

Deformation of Au Nanoparticles — ●Andreas Kelling, Burkhard Roos, and Cynthia A. Volkert — Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen

Compression experiments and TEM investigations have been performed on Au nanoparticles with diameters between 80 and 250 nm in an effort to understand nucleation and motion of dislocations in small volumes. TEM images of the 80 nm nanoparticles confirm that they are twinned in their as-received condition, but that the twins can be annealed out by heating to 400°C. Compression of the 250 nm diameter particles with a flat punch in a nanoindenter gives reproducible force-displacement curves, allowing controlled deformation of the nanoparticles to the desired strain. In preparation for TEM investigations of the deformed nanoparticles, compression tests have been performed on 80 nm diameter nanoparticles placed on a TEM-transparent SiN membrane. By investigating the stored dislocations in the deformed nanoparticles, it is hoped that insights will be gained into the mechanisms that lead to the high strength of sub-micrometer metal specimens.

MM 26.23 Tue 14:45 Poster C

SPM Studies of Dislocations in Deformed Au Thin Films — ●Sönke Schmidt[1], Alissa Wiengarten[1,2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]now at TU Berlin

The high strength of metal thin films relative to bulk materials is attributed to the inhibition of dislocation activation in small volumes, but the exact mechanisms are not clear. Studying dislocation-controlled deformation of thin films requires high resolution techniques such as TEM or SPM. In contrast to in-situ deformation in the TEM, in-situ SPM investigations do not require special sample preparation and provide quantitative Burgers vector information. However, they have poorer time resolution and can only image dislocations where they intersect the surface. In this study atomically flat gold thin films of about 100 nm thickness and a grain size of about 400 nm, produced by a template method on glass substrates, were investigated both in STM and AFM. Deformation of the films was performed by indentation of the tips into the sample surface. For future studies, these thin films will be transferred to deformable substrates, where they will be used for in-situ tensile test during AFM imaging.

MM 26.24 Tue 14:45 Poster C

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

The deformation behavior of nanoscale metals differs from that of bulk metals, showing in particular an increase in strength with decreasing size. The aim of this study is to determine the deformation process and strength of high quality single crystal Au nanowires using in-situ tensile testing in the SEM. Nanowires with diameters between 75 and 250 nm are mounted in a tensile setup using a micromanipulator and Pt deposition. The force on the wires is measured using a capacitive MEMS device during displacement controlled loading with a piezoelectric actuator. First results on a 180 nm diameter nanowire show homogeneous deformation up to ≈10% strain, followed by localized deformation and ductile rupture. Stress-strain curves and deformation morphologies for various diameter wires will be presented and interpreted in terms of in-situ TEM observations of dislocation activity obtained from the same wires in a separate study.

MM 26.25 Tue 14:45 Poster C

Automated dislocation detection in atomistic simulations — ●Alexander Stukowski, Jonathan Schäfer, and Karsten Albe — FB Materialwissenschaft, TU Darmstadt, Germany

We present a novel method that allows us to directly extract dislocation lines and their associated Burgers vectors from atomistic simulations. Our dislocation detection algorithm is based on an automated Burgers circuit analysis to trace dislocation cores followed by a vectorization step, thereby achieving the transition from the atomistic system to a discrete dislocation representation.

The dislocation analysis can be efficiently performed on-the-fly during molecular dynamics (MD) simulations with a high time resolution. This enables the investigation of rapid dislocation processes, whose observation was otherwise impeded by other crystal defects or simply by the huge amount of data produced by large-scale MD simulations.

Our analysis method can reliably detect perfect, partial, and twinning dislocations. For the first time, the dislocation density in MD simulations can now directly be quantified. In principle, even more comprehensive data not accessible before can be extracted, including dislocation mobility and dislocation reactions.

The new analysis method is applied to large-scale deformation simulations of nanocrystalline metals to study the density and character of dislocations as a function of strain. Being able to directly visualize and measure dislocation activity gives new insights into the interplay of grain-boundary mediated processes and dislocation plasticity in such materials.

MM 26.26 Tue 14:45 Poster C

Thickness Effects in Very High Cycle Fatigue Behavior of Cu Films — ●Clemens Trinks, Felix Hebenstreit, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

It has recently been established that decreasing the thickness of metal films leads to an increase in fatigue life and a change in fatigue damage morphology. This has been correlated with the high strength of thin films and attributed to their limited dislocation activity. The current research extends fatigue studies below 100 nm film thickness and to ultra high cycle numbers. Such studies are of great relevance for predicting the reliability of metal components used in micro- and nanotechnology, where they often experience repeated, low-level mechanical or thermal-mechanical loading. A resonant cantilever method has been developed using an AFM to test and monitor the fatigue behavior of

Cu films with thicknesses between 20 nm and 2 μm. Strain amplitudes up to 0.1 % and cycle numbers up to 10^{10} have been achieved. First results from a 200 nm thick film show evidence of narrow extrusions parallel and next to twin boundaries, as well as cracking and grooving at grain boundaries. This damage is similar to what is observed in low cycle fatigued films of similar thickness, giving first indications that the mechanisms of damage formation are determined predominately by the film thickness and not by the strain amplitude.

MM 26.27 Tue 14:45 Poster C

Strukturelle Umwandlungen von Niederdruckpolyäthylen bei mechanischer Beanspruchung — •Heinz Hans Walter Preuss — Hameln

Es werden die bislang weitgehend unbeachtet gebliebenen Ergebnisse der elektronenmikroskopischen Untersuchung [1] struktureller Umwandlungen von Proben aus Niederdruckpolyäthylen bei mechanischer Beanspruchung vorgestellt. Gezeigt wird, dass die mit dem Faltungsmodell nach Keller [2, 3, 4] gedeuteten Lamellen sich mechanisch voneinander trennen lassen, indem galvanisch mit Kupfer verstärkte Aufdampfschichten aus Gold von der Oberfläche sphärolithisch aus der Schmelze erstarrter Polyäthylenproben abgezogen werden. Mit direkten elektronenmikroskopischen Durchstrahlungsuntersuchungen lässt sich zeigen, dass die sphärolithische Struktur dünner Polyäthylenhäutchen sich beim Zerreißen übergangslos in Faserstrukturen umwandelt. Beim makrospröden Bruch massiver Polyäthylenproben bei Raumtemperatur und bei *195oC lässt sich sowohl die Umwandlung in Faserstrukturen als auch dass Erreichen der Schmelztemperatur bruchflächenmorphologisch nachweisen. Literatur: 1 A. Keller, Phil. Mag. /8/ 2, (1957), 1171 2 H. H. W. Preuß, Dissertation, Leipzig 1963 3 H. H. W. Preuß, physica status solidi, 3 (1963), Nr. 3, K109 ff. 4 H. H. W. Preuß, Plaste und Kautschuk, 10 (1963) Nr. 6, 330 ff.

MM 26.28 Tue 14:45 Poster C

Elastic: A program for calculating elastic constants for arbitrary lattice types based on ab-initio total energies — •Rostam Golesorkhtabar[1,2], Jürgen Spitaler[1,2], Peter Puschnig[2], and Claudia Ambrosch-Draxl[2] — [1]Materials Center Leoben Forschung G.m.b.H, Rosegger-str. 12, 8700 Leoben, Austria — [2]Montanuniversität Leoben, Franz-Josef-str. 18, 8700 Leoben, Austria

Detailed informations about elastic properties play a key role in material science and technology. On an atomistic level, this information is represented by the elastic tensor. We have present Elastic, a code that is able to calculate the full elastic tensor for any crystal structure from ab-initio total energies. For this purpose, structure files with special distortions corresponding to the lattice type are created. Then the total energies of all structures are determined from ab-initio calculations within density-functional theory, which are then fitted to the applied strains in order to get all independent elements of the elastic tensor. Based on the elastic tensor our program calculates the elastic compliances, the bulk, shear and Young moduli and the Poisson ratio. By using both, the Voigt and the Reuss averaging, the ab-initio results are related the elastic properties of polycrystalline samples. From symmetry considerations all space groups can be classified into 9 types differing in the number of independent components of the elastic tensor. We have tested our program for one representative of each class, using total energies obtained with the full-potential linearized augmented plane wave code WIEN2k, and compare the results with experimental data from literature.

MM 26.29 Tue 14:45 Poster C

Nanoantennae from high melting point transition metal nanowires — •Litty Varghese Thekkekara[1], Andreas Erbe[1], Diedrich A Schmidt[2], Martina Havenith[2], and Achim W Hassel[1] — [1]Max-Planck Institute für Eisenforschung,Düsseldorf — [2]Lehrstuhl für Physikalische Chemie II, Ruhr University, Bochum

Due to their optical properties, nano metallic objects attract considerable attention in various fields of nanotechnology, such as thermal emitters, sensor applications, and analytical bioscience.

Here, nanowires were prepared by electrochemical etching from directionally solidified eutectic alloys (NiAlX, X =Mo, Re, W) and transferred to infrared-transparent substrates, mainly silicon.We have performed optical and morphological characterization of single, high melting point transition metal nanowires (rhenium, molybdenum and tungsten) with high aspect ratios and a thin protective oxide layer. Nanowire morphologies were confirmed using scanning electron microscopy as well as atomic force microscopy. The length of the wires is ˜100μm,at a width of ˜400nm.

Optical properties were measured using infrared micro spectroscopy. Small metal nanostructures with high aspect ratio do normally show a strong antenna-like longitudinal plasmon mode at a wavelength λ ˜ 2L (L- length). Due to the length of the wires studied here, this mode is expected to be excited in the far infrared wavelength range.

MM 26.30 Tue 14:45 Poster C

Electronic Properties of Graphene Nanoribbons — •Ezgi Erdogan and Gotthard Seifert — Theoretische Chemie, TU Dresden, 01062 Dresden

The aim of present work is to review the electronic properties of Graphene nanoribbons (GNR) with the density functional tight binding method (DFTB) based on molecular dynamics (MD) simulation in the NVT ensemble for investigating energy gaps, defect area, strain effect and to understand switching between metallic and semiconducting properties. MD simulations are performed on Armchair GNR (AGNR) with (12,7,196) and (17,7,266) indexes and Zigzag GNR (ZGNR) with (20,9,198) and (22,9,216) indexes. The indexes (a,b,c) refer to 'a' - the width in number of carbon atoms, 'b' - the unit cell and 'c' - the total number of atoms in the configuration of the graphene sheet. The Graphene edges are saturated by hydrogen atoms. AGNRs are always semiconducting. The AGNR(12) has a 0.7 eV gap. During stretching process, one or two C-atom chains remain between two graphene halves. DOS pretends a switch to metallicity at a strain of 16%, but for the chain of single carbon atoms a band gap is visible in local density of states (LDOS). For AGNRs no change from semiconducting to metallic behavior for any value of strain is observed in transport calculations with a Green's function method. In contrast, ZGNRs remain conducting.

MM 26.31 Tue 14:45 Poster C

Aggregation of carbon in a H_2 atmosphere investigated by ReaxFF-molecular dynamics simulations — •Norbert Lümmen — University of Bergen, Department of Physics and Technology, Allégaten 55, 5007 Bergen, Norway

Controlled manufacturing of very pure carbon nanoparticles (Carbon Black) can be achieved by, for example, thermal decomposition of gaseous precursors like acetylene or methane. A large quantity of molecular hydrogen is produced during the decomposition process.

We have investigated the aggregation process of carbon molecules and hydrocarbons from carbon atoms in an atmosphere of H_2 at different temperatures, densities and initial amount of H_2 by molecular dynamics (MD) simulations. The calculation of interatomic forces within the MD-simulations was based on the Reax Force Field (ReaxFF).[1]

The growth of molecules and their compositional changes were followed up to 4 ns of simulation time. The developing number of ring structures based on carbon atoms was analysed by the shortest-path ring method.[2] Formation of carbon catenates and hydrocarbons of different sizes was observed. A decreasing amount of initial H_2 allows the aggregation of pure carbon molecules up to 30 atoms. Hydrogen atoms are found along and at the ends of these carbon chains in all types of systems. These linear molecules eventually aggregate to larger ones in which networks of rings of carbon atoms can be found.

[1] van Duin et al., J. Phys. Chem. A 105, 9396 (2001).

[2] Franzblau, Phys. Rev. B 44, 4925 (1991).

MM 26.32 Tue 14:45 Poster C

Mechanical Characterization of Layered Nanocomposites — •Inga Knorr, Susanne Seyffarth, Tobias Liese, Hans-Ulrich Krebs, and Cynthia A. Volkert — Institut für Materialphysik, Universität Göttingen

Multilayer thin films with dimensions at the nanometer scale represent a technologically important class of materials which can offer improved mechanical properties as a result of composite and size effects. The samples studied here consist of Cu/PMMA- and Ti/ZrO_2-multilayer films produced using pulsed laser deposition. Mechanical characterization is performed in a nanoindenter using Berkovich indentation as well as micro-compression tests on columns machined from the films with a focused ion beam microscope. Furthermore, the morphology of the samples in the undeformed and deformed states is investigated with SEM and TEM. The goal of the studies presented here is to gain information about the size-dependence of the layer mechanical properties as well as to identify deformation and failure mechanisms in multilayered samples. Details about the mechanical properties of films with layer thicknesses between 5 and 1000nm will be presented. The dependence of mechanical behavior and deformation morphology on layer dimensions will be discussed.

MM 26.33 Tue 14:45 Poster C

Structural and electrochemical properties of mixed transition metal phospho-olivine systems — •Michaela Memm, Peter Axmann, and Margret Wohlfahrt-Mehrens — Zentrum für Sonnenenergie- und Wasserstoff-Forschung Helmholtzstraße 8 89081 Ulm

lithium iron phosphate LiFePO4 shows a very good cycling stability at a potential of 3.5 V vs. Li/Li+ with a specific capacity of up to 160 mAh/g at room temperature. the potential and other properties of the phospho-olivines can be influenced by substituting other transition metals, such as manganese, cobalt and nickel, for iron. the transition metal phospho olivines can form solid solutions, among which LiFexMn1-xPO4 is a well known system. In this work, we prepared and characterized binary and ternary series of phospho olivines with M = Co, Mn, Fe, Mg. the systems form solid solution series LiCo1-xMxPO4 for M = Fe, Co and LiMgxFeyMn1-x-yPO4. The particle morphology is strongly influenced by M. A two step potential characteristic is observed for the mixed systems LiCo1-xMxPO4 and LiMgxFeyMn1-x-yPO4 with the single steps occurring on potential close to those of the pure end members. Significant potential shifts can be observed depending on the composition. We found high capacity yields for the Mg containing samples

MM 26.34 Tue 14:45 Poster C

Resistance measurements on a single nanoparticle and nanoparticle ensembles — •Ivan S. Titov, Marina Spasova, and Michael Farle — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany

In this work the resistance of 18 nm iron oxide nanocubes was measured using Scanning Tunneling Microscope mounted inside of Transmission Electron Microscope (TEM-STM technique). Chain-like structures consisting of the arbitrary numbers of the cubes were built using tungsten STM tips. The process of the chain formation was visualized in TEM. Voltage-current curves for a single nanocube and nanocube chains were recorded in a contact STM mode using gold and tungsten tips. Correlation of electrical properties with the structure and the chain morphology as well as influence of contact resistance and deformation of the samples on measured resistance values are discussed. The work is supported by DFG/SFB 445.

MM 26.35 Tue 14:45 Poster C

Near Surface Lattice Relaxation in Transition Metal Nanoparticles — •Björn Bieniek, Darius Pohl, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany

The near-surface lattice relaxation of transition metal alloy nanoparticles is investigated. Recent results show that CuAu and FePt particles show a pronounced lattice expansion of about 10% at their surface. Here, MD simulations indicate that the segregation of the heavier elements (Au, Pt) leads to the experimentally observed lattice expansion. However, surface-sensitive XAS and PES have revealed the presence of oxygen in the surface layers of FePt particles which could in turn contribute to and/or cause the expansion of the lattice. To investigate the influence of oxygen on the near-surface lattice expansion, FeNi particles are investigated. FeNi is much more susceptible to oxidation than CuAu and FePt. In contrast to the latter, abberation-corrected high resolution TEM on FeNi particles reveals that metallic particle cores are surrounded by crystalline oxide shells. Almost no lattice relaxation is observed in the metallic core, and the interface between the metal and the oxide is atomically sharp. Both, defects due to the lattice mismatch at the interface and a significant lattice relaxation are *only* observed in the oxide shell. MD Simulations and HRTEM contrast simulations of FeNi nanoparticles are presented to confirm the experimental results.

MM 26.36 Tue 14:45 Poster C

Adjusting the Size of Nanochannels in Silicon and Silicon Oxide Samples — •René Berwanger and Rolf Pelster — FR 7.2 - Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have prepared free-standing porous silicon layers by electrochemical etching of heavily p-doped silicon wafers. Pore size and porosity are analysed via nitrogen isotherms. With increasing etching time the thickness of the samples, the average pore radius and the porosity increase (r = 3 nm - 7 nm). Completely oxidized and transparent samples are obtained by heat treatment. This procedure does not affect the average pore radius although the total sample volume increases. Such a decrease of porosity can be explained with a simple model. These samples where used for measurements on confined n-alcohols. For some short-chain alcohols, which crystallize under normal condition, the confinement induces a glass transition.

MM 26.37 Tue 14:45 Poster C

Nanocrystalline $LiFePO_4$ Prepared by Mechanochemical Route — •Vladimir Šepelák[1], Sylvio Indris[1], Klaus Dieter Becker[2], Wolfgang Bensch[3], and Paul Heitjans[4] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Braunschweig University of Technology, Braunschweig, Germany — [3]Christian-Albrechts-University Kiel, Kiel, Germany — [4]Leibniz University Hannover, Hannover, Germany

Among the typical Li ion battery cathode materials, $LiFePO_4$ of the phospho-olivine family is particularly interesting due to its high power density, low cost, and environmental compatibility. Taking into account a nonequilibrium state of complex oxides prepared by mechanochemical methods [1], an enhanced electrochemical performance may be anticipated in such 'interface-controlled' materials.

In the present work, nanocrystalline $LiFePO_4$ with an average particle size of about 10 nm was prepared via far-from-equilibrium mechanochemical processing of the bulk $LiFePO_4$. HR-TEM studies revealed a nonuniform structure of $LiFePO_4$ nanoparticles consisting of an ordered core surrounded by a disordered surface shell/interface region. A comparative ^{57}Fe Mössbauer spectroscopic study of bulk and nanocrystalline $LiFePO_4$ revealed that the near-surface layers of phosphate nanoparticles are disordered due to the strongly distorted geometry of the FeO_6 octahedra. Quantitative information on hyperfine parameters of the nonequilibrium $LiFePO_4$ nanophase is obtained.

The work is supported by the DFG (SPP 1415).

[1] V. Šepelák et al., Chem. Mater. 21 (2009) 2518.

MM 26.38 Tue 14:45 Poster C

Finite-Size effects in GaN nanoparticles studied by a novel dynamic-charge transfer potential — •Manuel Diehm, Peter Agoston, and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, 64287 Darmstadt

Nanoparticles of compound semiconductors exhibit a number of peculiar properties, including phase transitions and unusual structural relaxations. Atomic scale modelling of such effects by quantum mechanical ab-initio calculations is, however, computationally too demanding, while classical potentials are limited to fixed charge models or computationally costly charge equilibration schemes. In this contribution, a novel dynamic charge-transfer bond-order potential (DCT-BOP) is applied, which opens the possibility to study larger ionic systems with variable charge states. The variability of the charges may carry great importance when modelling nanoparticles, since a reduction in the charge state of an ion can mitigate the impact of missing Coulomb interactions at surfaces or defects and change the energetics of relaxation. Here, we present calculations on Gallium Nitride nanoparticles using the DCT-BOP in comparison to a conventional bond-order potential and a pure Coulomb/Buckingham Potential. We examine the size dependence of charge states, relaxation energy gain and the interplay of surface and bulk contributions.

MM 26.39 Tue 14:45 Poster C

Low Energy Excitations in Semiconductor Nanoparticles — •Andreas Hartmann[1], Darius Pohl[1], Ludwig Schultz[1], Stephen Hickey[2], Alexander Eychmüller[2], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]TU Dresden, Physical Chemistry and Electrochemistry, Bergstr. 66b, D-01062 Dresden, Germany

Low energy excitations such as plasmons or excitons and also the semiconductor band gap usually depend strongly on the dimensionality and the size of the material. As a consequence, the control of various electronic properties of semiconductor nanoparticles by merely controlling their size is since long a vital research field. The vast majority of the investigations is, however, focussed on characterising the properties of particle ensembles, and only little work is so far dedicated to the correlation of size, structure, and electronic properties in individual isolated particles. Modern aberration-corrected HRTEM in combination with local EELS provides an effective tool to investigate such correlations. The potential of using HRTEM with a monochromated electron source at low acceleration voltages offers new opertunities to characterize low energy excitations with high energy and spatial resolutions. Here, the effective suppression of Cerenkov radiation backgrounds upon reducing the acceleration voltage and the gain in energy resolution by using a monochromated beam is largely beneficial to low energy EELS. The potential and the limitations of this method are explored for the example of colloidal wide band gap Zn-O nanoparticles.

MM 26.40 Tue 14:45 Poster C

Phase-field simulation using the Calphad method — •Sebastian Schulz, Abhik Choudhury, and Britta Nestler — Institute of Materials and Processes, Karlsruhe, Germany

The strength of the phase-field method to simulate material alloy systems has been demonstrated over the years. This requires the knowledge of the Gibbs-free energy of the phases involved in the transition. The Calphad method involves the calculation of phase diagrams of multi-component systems, using datasets generated through comparative studies with experiments and density functional theory calculations. This methodology has gained popularity for use in simulations and experimental studies, as this includes a creditable collection of the Gibbs-free energies of a number of material systems. Databases are available for most binary systems, and a number of ternary systems of technical interest. In the present study, we build the methodology for the direct use of the databases in the simulation of material alloys, using the phase-field method. In particular, we investigate the Al-Si system, given the wide range of microstructures possible and its significance in the industry.

MM 26.41 Tue 14:45 Poster C

Crystallization and Phase Separation of $Si_{1-x}C_x$ (x = 0.33) Films — •Kai Volgmann[1], Wolfgang Gruber[2], Harald Schmidt[2,3], Wolfgang Maus-Friedrichs[1,3], Udo Geckle[4], and Michael Bruns[4] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, D-38678 Clausthal-Zellerfeld — [2]Institut für Metallurgie, AG Materialphysik, TU Clausthal, D-38678 Clausthal-Zellerfeld — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, D-38678 Clausthal-Zellerfeld — [4]Institut für Materialforschung III, Forschungszentrum Karlsruhe GmbH, D-76344 Eggenstein-Leopoldshafen

Microstuctural changes during annealing of amorphous silicon carbide with varying silicon to carbon ratios are of considerable interest for tailoring of material properties in view of technical applications. We investigated phase separation and crystallization behaviour of magnetron sputtered amorphous $Si_{1-x}C_x$ films (x = 0.33) with a thickness of 1.4 μm deposited on Si substrates using XPS, GI-XRD and SIMS. For as deposited samples XPS confirm a Si/C ratio of 2:1. After annealing at 700 °C for 30 min the samples are still amorphous but XPS reveal a Si/C ratio of 1.33. The information depth of XPS is about 10 nm. During isothermal annealing at higher temperatures between 1200 and 1350 °C GI-XRD shows first the simultaneous formation of crystalline Si and nanocrystalline SiC. Further annealing leads to a continuous decrease and complete vanishing of crystalline Si, while the amount of SiC increases until fully crystallization. The temperature dependence and possible explanations of this effect are discussed.

MM 26.42 Tue 14:45 Poster C

Crystallization kinetics of phase change materials — •Andreas Kaldenbach, Sebastian Gabel, Carl Schlockermann, Martin Salinga, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase-change materials are one of the most promising candidates for future memory technology applications and are presently considered to replace FLASH-Memory or even DRAM. The non-volatility of the stored data is a key feature of these phase-change memories, which is enabled by a permanent structural rearrangement: the switching between a highly resistive amorphous state and a low resistance crystalline one. The fundamental mechanism of crystallization in these materials is still not fully understood. That's why a comprehensive investigation of the temperature dependence of crystal nucleation and growth is highly desirable. However, within the temperature regime between the glass transition temperature and the melting point, phase-change materials possess an extremely fast crystallization speed. Therefore a new optical in-situ tester has been assembled to tackle this challenge on a nanosecond timescale. It uses a pulsed laser to thermally induce the switching and a probe laser to measure the changing reflectivity during the switching process. The measurement principle is demonstrated using AgInSbTe, a typical phase change material known from optical data storage.

MM 26.43 Tue 14:45 Poster C

Simulations of the martensitic phase transition in NiTi — •Daniel Mutter and Peter Nielaba — Physics Department, University of Konstanz, 78457 Konstanz, Germany

In this work, molecular dynamics simulations of the martensitic phase transformation of NiTi are performed, which occurs between the low-temperature B19' structure and the high temperature B2 structure. This effect is the reason for the shape memory behaviour and the extraordinary superelasticity of NiTi, which make it one of the most commonly used shape memory alloys in engineering.

In order to explore the possibility to use these effects at the nanoscale, the simulations were carried out in a range of about 1000 - 4000 particles, with a potential arising from the tight binding model in the second moment approximation ([1]).

By analyzing the deformation of the simulation box and the crystal structure during a heating-cooling process, it is shown, that the B19' structure is stable at low temperatures and that the phase transition occurs at about 310 K for equiatomic NiTi. Further results show an extreme concentration dependence of the martensitic transition temperature, as well as the behaviour of the Gibbs free energy during the phase changes.

Because of a few not well reproduced experimental facts, first simulations with an improved potential ("modified embedded atom method" [2]) are presented.

[1] W. S. Lai, B. X. Liu, J. Phys. Cond. Mat. **12**, L53-L60 (2000).

[2] Y.-M. Kim *et al.*, Phys. Rev. B **74**, 014101 (2006).

MM 26.44 Tue 14:45 Poster C

Molecular Dynamics Simulations of Laser Ablation in orthorhombic $Al_{13}Co_4$ — •Steffen Sonntag, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

Femtosecond laser ablation of the Aluminum-Cobalt alloy $Al_{13}Co_4$ is investigated. For the simulations of the lattice ions we use molecular dynamics, while for the time evolution of the electron-temperature a generalized heat-conduction equation is solved by a finite difference scheme. Energy transfer between the subsystems is allowed by an electron-phonon coupling term. This combined treatment of the electronic and atomic systems is an extension of the well known two-temperature model [1]. The alloy shows large structural affinity to decagonal quasicrystals, which have an *in-plane* five-fold symmetry, while in perpendicular direction the planes are stacked periodically. As a consequence we observe slight anisotropic melting behavior.

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

MM 26.45 Tue 14:45 Poster C

Seed induced nucleation in colloidal model systems under microgravity — •Patrick Wette[1] and Hans Joachim Schöpe[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — [2]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz

Understanding the process that drives an under cooled fluid to the crystal state is still a challenging issue for condensed matter physics and plays a key role designing new materials. Crystallization undergoes crystal nucleation, growth and ripening. The crystallization kinetics and the resulting polycrystalline morphology are given by a complex interplay of these mechanisms. A great deal of progress has been made in recent years using colloidal suspensions as model system studying crystallization. We here present systematic measurements of the crystallization kinetics of a charged colloidal model system adding small amounts of seeds using time resolved scattering techniques. Large seeds show strong sedimentation under gravity even on the timescale of the crystallization process. To avoid this problem we performed our measurements under micro gravity during parabolic flights. We report how the seeds size and structure affect crystal nucleation and growth as function of meta stability giving the possibility to modify the crystallization process.

MM 26.46 Tue 14:45 Poster C

Phase transitions of colloidal monolayers on decagonal light induced substrates — Günther Gera, •Thomas Bohlein, Jules Mikhael, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Two dimensional phase transitions remain of high interest to a broad scientific community. According to KTHNY theory, melting in 2D occurs via two sequential defect-driven phase transitions. In this context colloidal systems, having a multitude of accessible interactions, offer a suitable way to investigate such phenomena in real space. Most of the work considered 2D colloidal systems with only mutual interactions, or in few cases interaction with underlying periodic substrate potentials. Here we report measurements of the complex phase behavior of a triangular colloidal monolayer in the presence of a quasiperiodic substrate potential acting via optical forces on the particles. Experimentally, it is created by interfering 5 laser beams. This potential, although not periodic, has a long range order and a decagonal rotational symmetry. At different potential strengths several phenomena are depicted. At low laser intensities, reorientation of the high symmetry axis of the crystal is observed. For higher intensities, we identify the typical geometrical point defects which mediate the transition to the quasicrystalline phase. Here, the structure factor exhibits the decagonal symmetry as expected. For certain densities, line defects lead to a transition to the Archimedean-like tiling phase.

MM 26.47 Tue 14:45 Poster C

Studies on phason flips by kinetic Monte Carlo simulations — •Hansjörg Lipp and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Stuttgart

Neutron scattering experiments [1] indicate that atoms in quasicrystals perform flips between split positions with typical time scales of picoseconds. On the other hand, Edagawa et al. have presented HRTEM images [2], where bright spots are flipping with periods of seconds or even minutes.

To explain this apparent discrepancy, we start from a structure model for d-Al-Cu-Co of Zeger et al. [3], where a ring of ten atoms can perform a jump by four consecutive single atom flips. By applying kinetic Monte Carlo simulations [4], we study how these collective flips, which occur in the different layers of the d-phase can lead to flips detectable by HRTEM on much lower frequency scales.

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

MM 26.48 Tue 14:45 Poster C

Vapour galvanizing (Sherardizing) of Copper with Zinc — •Dietbert Wortelen[1], Hartmut Bracht[1], Frank Natrup[2], and Wolfram Graf[2] — [1]Westfälische Wilhelms-Universität Münster, Germany — [2]Bodycote Wärmebehandlung GmbH, Sprockhövel, Germany

Using a vapour galvanizing technique called Sherardizing we investigated the growth kinetics and coefficients of zinc copper phases. For this purpose polished (OFHC)-copper plates and zinc powder have been sealed in quartz ampoules under inert gas atmospheres and annealed at a temperature range between 300 and 410°C. In order to study the coating thickness and the phase composition, cross sections were prepared, which have been analyzed by means of optical microscopy and scanning electron microscopy. We were able to demonstrate that the coating thickness is a function of the parabolic time law and that the formed coatings are composed of two layers referring to the ordered beta-CuZn and gamma-Cu5Zn8-phases. To enhance the coating quality, small amounts of ZnCl2 were added to the zinc powder. It was observed that the coating thickness decreased with increasing ZnCl2. Experiments with variable Ar-pressure demonstrated a reduced coating growth with increasing pressures. Further measurements with ZnCl2 were performed to check whether an electrochemical mechanism is involved in the coating process.

MM 26.49 Tue 14:45 Poster C

Hydrogen absorption in Gd thin films and islands — •Sara Wanjelik, Georg Oeltzschner, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

The absorption process of hydrogen in thin Gd(0001) films deposited on a W(110) substrate has been investigated by means of scanning tunneling microscopy (STM) and spectroscopy (STS). The adsorption as the previous step is imaged using the fact that clean and well-ordered Gd surfaces exhibit a highly localized surface state near the Fermi edge which is suppressed due to the adsorption of hydrogen. The surface state reappears after the subsequent diffusion of hydrogen into the bulk material. Thus, we are able to observe the temporal development of the absorption process.

In this contribution we will discuss the absorption behaviour for different layer thicknesses to determine the influence of the respective bulk material because the creation of GdH_2 results in a lattice expansion of about 14%. Due to the adherence of the film on the substrate this expansion occurs only in the perpendicular direction. This is different for free standing nanoislands which are only clamped at the interface. Thus, investigations concerning the absorption behavior are also performed on the size dependence of Gd islands to compare these results with those from thin films.

MM 26.50 Tue 14:45 Poster C

Properties and stability of hydrogen sensors based on magnesium-iron thin films — •Gunther Haas, Jennifer Stiebich, Andreas Laufer, Marc Dietrich, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Thin magnesium-iron films, capped by a catalytic Pd layer, were prepared by RF diode sputtering. Upon exposure to hydrogen the films show reversible changes in the optical reflection and electrical resistivity. These switching effects can be use to detect hydrogen gas. We investigated the influence of the sputter parameters and the layer thickness on the sensor performance in air and argon atmosphere. Due to the layer optimisation the sensitivity could be extended from 4% to less than 1000 ppm hydrogen in air and response times faster then 10 s were obtained. Considering the stability and durability of the sensors, the long-term stability is restricted by the interdiffusion of Mg into the Pd layer and fractional oxidation. Therefore we investigated the effect of an additional metal layer which allows hydrogen diffusion but suppresses the oxidation and/or the interdiffusion of Mg.

MM 26.51 Tue 14:45 Poster C

Chemical trends of the solution enthalpy of hydrogen in 3d transition metals in dilute limit, derived from first principles — •Ugur Aydin[1], Lars Ismer[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung GmbH — [2]University of California, Santa Barbara

Hydrogen embrittlement is a general phenomenon, which has already been observed in several transition metals and which is of high technological relevance. Despite many investigations of related mechanisms, a purely theoretical prediction how much a material of a certain chemical composition is affected by hydrogen embrittlement is still not possible. However, there is no doubt that the hydrogen solution enthalpy, ΔH, and its dependence on the crystal strain is a decisive criterion. We therefore performed a detailed ab initio investigation of the ΔH dependence on the band filling in 3d transition metals under comparable conditions. For this purpose, density functional theory within the GGA approximation was employed. Zero point vibrations have been taken into account using the Einstein model. The analysis revealed a universal dependence on the crystal lattice constant, with a material specific interplay of chemical and strain contributions. We compared our first principles findings with semi-empirical rules for the hydrogen solubility stated by Griessen et *al.* [PRB **38**, 3690 (1988)] and confirmed that out of the parameters discussed there (electronic density, bandwidth of the d-band, atomic spacing) the distance of nearest neighbouring host atoms has the most systematic influence on ΔH.

MM 26.52 Tue 14:45 Poster C

Hydrogen absorption behavior of nano-crystalline Mg thin films — •Helmut Takahiro Uchida, Astrid Pundt, and Reiner Kirchheim — Institut fuer Materialphysik, Friedrich-Hund-Platz 1, D-37077, Goettingen, Germany

Hydrogen absorption behavior of nano-crystalline Mg thin films are electrochemically investigated at room temperature. 20nm Pd-capped nanocrystalline Mg films of different thicknesses were prepared in an UHV chamber, by means of ion beam sputter deposition under Ar-atmosphere at the pressure of 2,5*10E-4 mbar. Nano-crystalline Mg films were deposited on Si (100) substrates for P-C-T measurements of hydriding, and on annealed Pd-substrates with thickness of less than 0.25mm for hydrogen permeation measurements. All the films were covered by a 20 nm thick layer of Pd in order to prevent oxidation. The influence of loading current density on hydrogenation property were observed by measuring electromotive force (EMF). Diffusion coefficient of hydrogen in nano-crystalline Mg thin films at room temperature are estimated at several hydrogen concentration, and the impact of grain boundary on hydrogenation property is discussed. XRD measurements using a Phillips X-Pert diffractometer with a Co-K alpha radiation were performed before and after hydrogenation in order to check the phase transition and change of texture in the sample.

MM 26.53 Tue 14:45 Poster C

Oxygen and silicon diffusion in mixed cation silicate glasses — •Kirsten Sunder and Hartmut Bracht — Institut für Materialphysik, Wilhelm-Klemm-Straße 10, WWU Münster

The impact of alkali (A) and alkaline-earth (M) ions on oxygen (O) and silicon (Si) diffusion in mixed cation silicate glasses of the composition aA2O-bMO-4SiO2 was investigated. In particular, the dependence of network former diffusion on the type of cations (A=Li,Na,K; M=Mg,Ca,K), the concentration of non-bridging oxygens (a=0.5,1,1.25; b=2a), and the alkali to alkaline-earth ratio (a=0,1,1.5; b=3-a) was determined. This study together with the work on the cation mobility [F.V. Natrup et al., Solid State Ionics 180 (2009) p. 109] provides a comprehensive understanding of the dynamics in this glass system.

MM 26.54 Tue 14:45 Poster C

Alternative contacting concept for ZnO nanostructures with regard to sensing applications — •Martin Gnauck[1], Ulrich Schröder[1], Raphael Niepelt[1], Carsten Ronning[1], and Rainer Adelung[2] — [1]Institute for Solid State Physics, Friedrich-Schiller-University Jena — [2]Institute for Materials Science - Functional Nanomaterials, Christian-Albrechts-University Kiel

Due to the direct band gap of 3.37 eV at room temperature and high surface-to-volume-ratios zinc oxide nanowires exhibit some promising properties for upcoming sensing applications. Studying the electrical and opto-electrical properties of single nanowires usually requires complex techniques like electron beam lithography or preparation via focused ion beam (FIB). Well established photolithography, however, is economically reasonable and allows fabrication of new nanostructure based devices on a much larger scale.

Here, we present a comparatively easy method for contacting one- and two-dimensional ZnO nanostructures and investigate their electrical properties with regard to possible applications as UV-light and gas detectors. Therefore, photolithography is used for pre-structuring and pre-contacting the VLS-grown nanowires and nanosails.

MM 26.55 Tue 14:45 Poster C

Polymer-Based Magnetoelectric Composites — •Kerstin Meurisch, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — Technische Fakultät, Institut für Materialwissenschaft, CAU Kiel

In magnetoelectric (ME) materials the change of an external magnetic field induces a change of the internal electric potential. Composites containing a magnetostrictive phase embedded into a piezoelectric matrix exhibit very high indirect ME coefficients compared to those direct ones of single phase materials. Furthermore, using piezoelectric polymers as matrices is advantageous, for example if high flexibility of the product is required or if the product is very sensitive to leakage currents in the matrix. Since polymers generally have a very small dielectric constant and a low Young's modulus, their ME coefficients exceed those of ceramic-based composites. Regarding the design of the composites, several microstructures are possible. The most prominent designs are laminates and particulate structures. Two approaches for the development of an polymer-based ME composite are presented: Firstly, as a basic step towards particulate composites, piezoelectric thin films of Nylon-11 were deposited via thermal evaporation. Secondly, laminates were fabricated by sputtering Cobalt onto a purchased piezoelectric Polyvinylidenfluorid(PVDF) foil. Preliminary results such as the effective piezoelectric coefficient of Nylon-11 and the effective ME coefficient of the laminates will be discussed.

MM 26.56 Tue 14:45 Poster C

Vapour phase deposition of ceramic-based granular nanocomposites for magnetoelectric applications — •Björn Gojdka, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — University of Kiel, Institute for Materials Science, Kaiserstraße 2, 24143 Kiel

The investigation of magnetoelectric materials has experienced a renaissance during the last decade due to promising new theoretical and experimental results and the technical potential of such materials [1]. However, up to now investigations of magnetoelectric granular nanocomposites, in which magnetostrictive clusters are embedded in a piezoelectric matrix, are scarce [2].

We report on the fabrication of granular magnetoelectric nanocomposites via combined rf and DC magnetron sputtering. Quasi-laminar systems, consisting of alternating layers of piezoelectric ceramic and layers of percolated magnetostrictive clusters were fabricated by tandem-sputtering. The deposition by co-sputtering of a BaTiO3 ferroelectric matrix containing clusters of Co on single-crystal SrTiO3 substrate was studied.

The structure was characterized by XRD. For the analysis of the composition and morphology of the composites TEM and SEM/EDX were utilized.

[1] C.W. Nan et al., Journal of Applied Physics 103, 031101 (2008)

[2] J. H. Park et al, Applied Physics Letters 92, 062908 (2008)

MM 26.57 Tue 14:45 Poster C

Ag-TiO2 nanocomposites for antibacterial and photocatalytic applications — Tomislav Hrkac[1], Venkata Sai Kiran Chakravadhanula[1], Nathalie Wohner[1], Vladimir Zaporojtchenko[1], •Thomas Strunskus[1], Dieter Garbe-Schönberg[2], and Franz Faupel[1] — [1]Institut für Materialwissenschaft-Materialverbunde, Christian-Albrechts-Universität zu Kiel, Kaiserstr. 2, 24143 Kiel — [2]Dept. of Geology/ ICPMS Lab, CAU Kiel, Ludewig-Meyn-Strasse 10, 24118 Kiel

Nanocomposites offer the possibility to combine the antibacterial property of Ag with the photocatalytic activity of TiO$_2$ in one material. Here TiO$_2$-Ag 2D and 3D nanocomposites were prepared by physical vapor deposition techniques allowing to varying many different morphologies. The antibacterial efficiency was studied by monitoring the silver release using ICP-MS. The optical structural properties of the composite was characterized by UV-Vis, XRD, HRTEM and XPS, and the photocatalytic activity was determined by UV illuminated dye photo degradation. Considering the different morphologies the correlation of photocatalytic activity and silver release will be discussed.

MM 26.58 Tue 14:45 Poster C

Experimental Thermodynamics and Phase Relations of New Anode Materials for Li-Ion-Batteries — •Hans Flandorfer, Klaus Richter, and Herbert Ipser — Institut für Anorganische Chemie / Materialchemie, Universität Wien, Wien, Austria

Li-Ion batteries have for long been recognized as an efficient way to store electric energy. For use in traction applications, however, these batteries have to meet several design criteria, such as number of charge/discharge cycles, energy density and safety.

The scope of SPP 1473 *WeNDeLIB* is the systematic investigation of materials interaction between the various materials used for cathode, anode, electrolyte and separators. The constitution of the relevant systems has been recognized as an important issue to understand the performance of the whole assembly.

Our Department has long lasting expertise in the field of phase diagram research and determination of thermodynamic properties. Together with other methods like EMF measurements and isopiestic vapor pressure measurements, all data required for thermodynamic modeling can be generated.

Our group will focus on the purely metallic anode materials. Co-Sn, Ni-Sn, Cu-Sn, and many others have been proposed as suitable materials. Thus, thermodynamics and phase relations of the respective ternary systems (Co,Cu,Ni)-Li-Sn will be investigated.

MM 26.59 Tue 14:45 Poster C

Electrochemical investigation of nanoscaled LiCoO$_2$ from different synthesis processes — •Carsten Jaehne, Christine Täschner, Andreia Ioana Popa, Rüdiger Klingeler, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden

Self-assembled nanoscaled cathode materials promise increased rate performance in Li-ion batteries. We report on the conventional and the microwave assisted hydrothermal synthesis of LiCoO$_2$ nanostructures. We discuss the effect of both synthesis processes as well as of the variation of the process temperatures between 120°C and 200°C and of different precursors on the morphology and electrochemical properties of the resulting material. Our electron microscopy, x-ray diffraction and magnetisation studies provide information about the phase, the morphology and the valency of the Co-ions. Cyclic Voltammetry and Galvanostatic Cycling techniques have been applied to evaluate the electrochemical performance.

MM 26.60 Tue 14:45 Poster C

Magnesium secondary batteries based on V$_2$O$_5$ cathodes — •Wiebke Lohstroh, Philipp Leufke, and Horst Hahn — Institute of Nanotechnology, Karlsruhe Institute of Technology, Postfach 3640, 76021 Karlsuhe, Germany

The development of high performance, reliable energy storage systems is a mandatory prerequisite if the use of fossil fuels shall be curtailed in mobile and stationary applications. Important parameters for any energy storage system are energy and power density as well as reliability, cycle life, safety and cost. Lithium ion secondary batteries are thought to be able to meet these demands and research activities have been intensified in recent years. An alternative pathway, which has only been explored little so far, is a secondary battery based on polyvalent ions,e.g. the Mg/Mg^{2+} redox couple. Mg is abundant and it is thought to be intrinsically safer than the Li analogue thus Mg based batteries could be a viable option for cost sensitive areas.

We will present first results on Mg secondary battery cells using a V_2O_5 cathode, Mg-metal anode and an organometallic electrolyte [1]. V_2O_5 electrodes made from powder show a reversible electrochemical response at potentials between 0 and 2 V vs Mg. However CV measurements indicate that discharge (i.e. Mg intercalation) occurs quite sluggish while during charging two distinct steps can be discriminated. First results on the electrochemical behavior of thin film V_2O_5 electrodes will also be presented.

[1] D. Aurbach, Z. Lu, A. Schechter, Y. Gofer, H. Gizbar, R. Turgeman, Y. Cohen, M. Moshkovich, and E. Levi, Nature 407, 724 (2000).

MM 26.61 Tue 14:45 Poster C

Blends of LiMn2O4 Spinel and LiNi0.8Co0.15Al0.05O2 for Advanced Lithium-Ion Batteries — •Hai-Yen Tran, Corina Täubert, Peter Axmann, and Margret Wohlfahrt-Mehrens — Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Helmholtzstrasse 8, D-89081 Ulm

Lithium manganese oxide spinel is a promising material for the positive electrode in lithium ion batteries due to the high abundance, low cost, non-toxicity, low irreversible capacity loss and high thermal stability. However, it suffers from relatively low discharge capacity, poor cycle life and poor electrochemical performance at elevated temperatures. Therefore, an interesting alternative would be to mix LiNi0.8Co0.15Al0.05O2 (NCA)and lithium manganese oxide spinel in defined ratios in order to compensate for their disadvantages each other. The aim is to obtain a material that could be comparable or even better than the conventional LiCoO2 with respect to discharge capacity, thermal stability and rate capability. In the present work we have evaluated the electrochemical performance of the mixed oxide electrodes by means of galvanostatic cycling with potential limitation. Blending the layered oxide (NCA) with manganese oxide spinel decreased the irreversible capacity loss and at the same time improved the rate capability of the electrodes. In addition, the manganese dissolution from the spinel structure was drastically reduced by NCA blending as well. The experimental results were compared to the theoretical calculations. The obtained results will be presented and discussed during the meeting.

MM 26.62 Tue 14:45 Poster C

Structure and negative thermal expansion in Cu(In1-xGax)(S, Se)2 — •Christiane Stephan[1], Susan Schorr[2], Denis Sheptyakov[3], and Hans-Werner Schock[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Solarenergieforschung, Glienicker Straße 100, 14109 Berlin — [2]Freie Universität Berlin, Fachbereich Geowissenschaften, Malteserstraße 74-100, 12249 Berlin — [3]Laboratory for Neutron Scattering, ETH Zürich & PSI Villigen, CH-5232 Villigen, Schweiz

Compound semiconductors like Cu(In1-xGax)(S, Se)2 are due to their superior optical and electronical properties successfully used as absorber layers in thin film solar cells. These compounds adopt the chalcopyrite type structure, which is characterized by a tetrahedrally coordination of the cations by anions and vice versa. One of the most intriguing properties of solids whose crystal structures are based on tetrahedrally coordinated ions is their negative thermal expansion. To verify this concept, in-situ neutron diffraction experiments in a temperature range from 290K to 1.5K were performed on Cu(In1-xGax)(S, Se)2 powder samples. The lattice parameters and linear thermal expansion coefficients were determined by Rietveld-Analysis of the neutron diffraction data applying the chalcopyrite structure as structural model and using the FullProf suite software package. Negative thermal expansion coefficients were observed for the Cu(In1-xGax)Se2 compounds, whereas the critical temperature, where alpha(a,c) becomes negative, varies with chemical composition.

MM 26.63 Tue 14:45 Poster C

Electrical properties of grain boundaries in Cu(In,Ga)(S,Se)$_2$ thin films for solar cells — •Jaison Kavalakkatt, Daniel Abou-Ras, Melanie Nichterwitz, Raquel Caballero, Björn Marsen, Thorsten Rissom, Thomas Unold, and Hans-Werner Schock — Helmholtz Center Berlin for Materials and Energy, Berlin, Germany

Electron-beam-induced current (EBIC) and electron backscatter diffraction (EBSD) in a scanning electron microscope are powerful tools to investigate the electrical and microstructural properties of grains and grain boundaries in Cu(In,Ga)(S,Se)$_2$ absorber layers in thin-film solar cells. For the present investigation, the Mo/glass stack was stripped off the remaining Cu(In,Ga)(S,Se)$_2$/CdS/ZnO heterojunction, in order to prepare a Cu(In,Ga)(S,Se)$_2$ surface with reduced roughness, leading to both, high-quality EBSD patterns and decreased number of topography artefacts in EBIC distribution images. In comparison to EBIC analyses on cross-section samples, the measurements on back-surfaces increase the number of accessible grain boundaries and therefore improve the statistics of their electrical properties. EBSD maps identify clearly the positions of the grain boundaries as well as allow for their classifications. Across various grain boundaries, profiles were extracted from EBIC distribution images. Corresponding simulation of these profiles provide values for minority-carrier diffusion lengths and recombination velocities at grain boundaries. The general result for Cu(In,Ga)Se$_2$ layers with various In/Ga ratios as well as Cu concentrations is a similar collection at grain interiors and $\Sigma 3$ grain boundaries and a reduced charge-carrier collection at non-$\Sigma 3$ grain boundaries.

MM 26.64 Tue 14:45 Poster C

Efficient simulation of plasmonic structures for thin film silicon solar cells — •Daniel Lockau[1,2], Sven Burger[2,3], Lin Zschiedrich[2,3], Frank Schmidt[2,3], and Bernd Rech[1] — [1]Helmholtz–Zentrum Berlin, Berlin, Germany — [2]Zuse–Institut Berlin, Berlin, Germany — [3]JCMwave GmbH, Berlin, Germany

Thin film silicon solar cells suffer from the disadvantage of a low absorption coefficient of silicon in important spectral regions. In the case of a flat multilayer cell layout a considerable part of the incident light is reflected back out of the cell due to the low absorber thickness. It is therefore desirable to introduce scattering elements that prolong the average photon path length inside the solar cell's absorber. Plasmonic structures are an upcoming area of research in this field. They might be better suited for optimization than other means of light trapping. The influences of periodic arrays of metal scatters on cell absorption can be very well assessed by different simulation methods.

We employ the finite element method for 3D simulations of Maxwell's equations. The setup for our simulations has been proposed by Rockstuhl et al. (C. Rockstuhl, S. Fahr, F. Lederer, *J. Appl. Phys.* 104, 123102 (2008)) who numerically studied absorption enhancement in a thin bulk of amorphous silicon due to scattering on a periodic array of silver discs. Using the same setup we show that our method is very time and memory efficient for the simulation of such plasmonic structures. Absorption enhancement is shown for wavelengths above 500 nm compared to the absorption without silver discs.

MM 26.65 Tue 14:45 Poster C

Structural characterization of AgGaSe$_2$ thin films grown by Chemical Close Spaced Vapor Transport (CCSVT) — •Christoph Merschjann[1], Barys Korzun[1,2], Susan Schorr[3], Thomas Schedel-Niedrig[1], and Martha Christina Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus — [3]Free University Berlin, Institute of Geological Sciences, Berlin, Germany

Thin films ($d \approx 3\ \mu$m) of n-type AgGaSe$_2$ thin films were successfully grown on glass and glass/molybdenum substrates using the technique of Chemical Close Spaced Vapor Transport (CCSVT). The structural characterization of the thin films was carried out by grazing incidence X-ray diffraction (GIXRD). The observed Bragg peaks belong exclusively to the chalcopyrite type structure. The lattice parameters and the atomic position of the anions were determined by Rietveld analysis of the GIXRD data. The structural refinement revealed also, that in the thin film only one phase, chalcopyrite type AgGaSe$_2$, is present.

The results are compared to those published for single crystalline AgGaSe$_2$. A comparative discussion of structural properties of chalcopyrite type compounds with different monovalent cations (Ag$^+$ vs. Cu$^+$) will round the presentation.

MM 26.66 Tue 14:45 Poster C

The Influence of wet-chemical smoothing on electronic properties of Si/SiO$_2$ interfaces prepared by UHV plasma oxidation — •Orman Gref, Bert Stegemann, Enno Malguth, Maurizio Roczen, Heike Angermann, and Manfred Schmidt — Silicon Photovoltaics, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

The successful application Si/SiO$_2$ interfaces for ultrathin oxides or nanostructures in third generation photovoltaics requires a minimum density of Si gap states. In order to achieve this goal, the influence of various wet-chemical pre-treatment procedures on the electronic properties of Si/SiO$_2$ interface was investigated. Structurally abrupt Si/SiO$_2$ interfaces were prepared under ultrahigh vacuum conditions by RF plasma oxidation of n-type Si(111) substrates with thermalized neutral oxygen atoms. A decrease the interface states was achieved by saturating dangling bonds through in situ RF hydrogen plasma passivation . The density of gap states at the Si surface and Si/SiO$_2$ interface was investigated by non-destructive and surface-sensitive surface photovoltage (SPV) experiments. Various sequences of wet-chemical oxidation and oxide removal steps in HF- or NH$_4$F solutions were successfully applied to reduce the substrate surface micro-roughness and surface state density. These optimised wet-chemical smoothing procedures yield a significant decrease in interface state densities of the subsequently prepared Si/SiO$_2$ interfaces D_{it}=1*10$_{12}$cm^{-2}eV^{-1}, compared to D_{it}=3.5*10^{12}cm^{-2}eV^{-1}, obtained after applying solely the standard RCA cleaning process and HF solution.

MM 26.67 Tue 14:45 Poster C

Minority carrier lifetime of InGaAsP and InGaAs absorbers for low bandgap tandem solar cells — •Nadine Szabó, B. Erol Sagol, Ulf Seidel, Klaus Schwarzburg, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH Hahn-Meitner-Platz 1 14109 Berlin

At present, III-V triple junction (3J) solar cells are achieving the highest conversion efficiencies (η=41.6%) worldwide. To improve the efficiency significantly, it is necessary to increase the number of junctions and to involve a subcell with an absorber layer in the band gap range of 1eV. We show on the example of the low band gap tandem cell how the choice of the materials, the quality of the bulk, the optimization of the band gap energies and the preparation of the critical interfaces are essential to build a high efficiency solar cell. A four-junction device can be realized by mechanically stacking of a GaAs-based GaInP/GaAs tandem cell with a InP-based InGaAsP/InGaAs tandem cell. We have grown InGaAsP and InGaAs layers lattice matched to InP substrates, and investigated the properties of the absorber bulk material. We will present time resolved photoluminescence measurements of low band gap InGaAs and InGaAsP double hetero structures (DHS). This technique is both sensitive for the quality of the bulk material within the DHS as well as for the interface preparation between barrier and bulk.

MM 26.68 Tue 14:45 Poster C

Electrical characterisation of oxide-pn-junctions under illumination — •Gesine Saucke[1], Benedikt Ifland[1], Constanze Thees[1], Jonas Norpoth[1], Jörg Hoffmann[1], Yimei Zhu[2], and Christian Jooss[1] — [1]Institute of Materials Physics, University of Göttingen, Germany — [2]Brookhaven National Laboratory, Upton NY, USA

Correlation effects in complex oxide materials should strongly affect the properties of a pn-junction with respect to energy conversion under illumination. As a model system of a photo-active oxide junction, epitaxial thin films of p-type Pr$_{1-x}$Ca$_x$MnO$_3$ (PCMO) were deposited on Nb doped SrTiO$_3$ (Nb-STO) single crystals. Low-resistance ohmic contacts on Nb-STO were obtained for deposited Ti or Al top layers, whereas high work function noble metals reveal non-linear IV characteristics. Since correlation effects, e.g. charge ordering in PCMO, takes place at lower temperatures, the electric characterization with and without illumination via IV curves was performed in a temperature range between 10 K and room temperature. A detailed characterization with respect to crystallographic structure, surface morphology, and interface intermixing was performed by means of TEM, AFM, SIMS and EELS. We found a small Ti-Mn exchange at the PCMO/Nb-STO interface which extends over a few lattice cells. In addition, we will present first results on p-type La$_{1-x}$Sr$_x$MnO$_3$ (LSMO) / Nb-STO based cells.

MM 26.69 Tue 14:45 Poster C

Comparative analysis of models for solute trapping in rapid solidification — •Ekaterina Abramova[1], Denis Danilov[2], Peter Galenko[3], Dieter Herlach[3], and Vladimir Lebedev[1] — [1]Udmurt State University, Faculty of Physics and Energetics, 426034 Izhevsk, Russia — [2]Karlsruher Institut für Technologie (KIT), Theoretische Biophysik, 76131 Karlsruhe — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Phase-field models (WBM- and EFKP-model [1,2]) are extended in the present work to rapid solidification in which local non-equilibrium phenomena occur in bulk phases and within the diffuse solid-liquid interface. The extended model is developed using a thermodynamic approach to fast phase transitions within a diffuse interface in a binary system [3]. We investigate solute trapping, which has been introduced to define the processes of non-equilibrium solute redistribution at the solid-liquid interface. The solute trapping effect in solidifying binary melts is compared with previous sharp-interface models and using the present extensions of WBM- and EFKP- phase-field models. This work is supported by RFBR Nos. 08-02-91957NNIO_a, 09-02-12110-ofi-m; ROSNAUKA No. 2009-1.5-507-007-002; DAAD No. A/08/81583; DFG No. HE 1601/19; DLR Agency under contract number 50WM0736.

[1] A.A. Wheeler, W.J. Boettinger, G.B. McFadden: Phys. Rev. E 47 (1993) 1893. [2] B. Echebaria, R. Folch, A. Karma, M. Plapp: Phys. Rev. E 70 (2004) 061604. [3] P. Galenko, D. Jou: Phys. Rev. E 71 (2005) 046125.

MM 26.70 Tue 14:45 Poster C

A phase-field model for polycrystalline grain growth on thin films — •Christian Mennerich, Frank Wendler, and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Polycrystalline grain growth on thin films is of high interest for catalytic active supports or molecular sieves (e.g. zeolites of the MFI-type). Growth competition between the grains determines the final structure of the film and therefore its properties. It is essential to understand the basic principles controlling the selection mechanisms. A phase-field model is presented to describe competitive grain growth on thin films in 2D and 3D. The model is derived from a free energy functional of Ginzburg-Landau type and supports different anisotropy functions to represent various crystal symmetries. The anisotropy is based either on surface energetic or kinetic considerations. As an example, we show results from coffin shaped crystal structures with a fixed aspect ratio competing on thin films. We focus on mechanisms related to the deviation of grain orientations from the film normal. This leads to the outgrowth and extinction of disadvantageously oriented grains, depending on their neighbourhood.

MM 26.71 Tue 14:45 Poster C

Anti-coarsening and complex dynamics of step bunches on vicinal surfaces during sublimation — •Marian Ivanov[1], Vladislav Popkov[2], and Joachim Krug[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str.77, D-50937 Köln — [2]Interdisziplinäres Zentrum für Komplexe Systeme, Rheinische Friedrich-Wilhelms-Universität Bonn, Römerstraße 164, D-53117 Bonn

Using morphological instabilities one can produce templates for nanoscale technology. One example of such an instability is step bunching, which splits a regular vicinal surface into regions of low and high density of monoatomic steps. The dynamics of the surface is described by the Burton-Cabrera-Frank model with boundary conditions provided by mass conservation at the steps. We consider a one-dimensional step train evolving in the presence of sublimation, step-step interactions and an Ehrlich-Schwoebel effect. We show that the interplay of sublimation and step-step interactions removes the conservation law for the crystal volume in the co-moving frame, which has been assumed in previous work [1,2]. As a consequence large step bunches are found to break up into smaller bunches of a characteristic size, and the monotonic coarsening dynamics of the volume-conserving model is replaced by a complex quasiperiodic pattern.

[1] V. Popkov, J. Krug, Europhys. Lett. 72, 1025 (2005) [2] V. Popkov, J. Krug, Phys. Rev. B 73, 235430 (2006)

MM 26.72 Tue 14:45 Poster C

Growth kinetics and morphology of silicon crystallites synthesized from metallic solution — •Thomas Teubner, Robert Heimburger, Nils Dessmann, Torsten Boeck, and Roberto Fornari — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin

The growth of large Si crystallites on amorphous substrates at low temperatures is highly desirable for fabrication of thin film solar cells but it remains a very challenging task. We use a low melting metallic solvent for Si seeding as well as subsequent growth. Supersaturation of solvent droplets for seed generation is reached via influx of Si from vapor and can be controlled by deposition rate. In contrast, expansion of Si seed crystal has been performed in a separate steady state solution growth equipment applying hereby a temperature gradient between vertically stacked feeding source, solvent, and substrate. The temperature difference of about 10 K enables continuous flow of solute towards substrate and thus provides the necessary supersaturation of solution around seed crystals. {111} and {110} facets are thermodynamically flat at 873 K. Even the experimental supersaturation is not sufficient to provoke kinetic roughness. An estimate of ledge free energy for two-dimensional nuclei suggests that the undercooling necessary for nucleation rates of 1 $\mu m^{-2}s^{-1}$ is 45 K for {111} and 18 K for {110} facets. Therefore, two-dimensional nucleation on {111} facets seems to be unlikely. The grown {111} faceted crystals are often twinned and partly exhibit hopper morphology. The latter can be explained by spreading of steps from apexes and edges and by spatial solute inhomogeneity.

MM 26.73 Tue 14:45 Poster C

Growth of para-hexaphenyl (6P) on silicon oxide by hot wall epitaxy — •Markus Kratzer, Quan Shen, and Christian Teichert — Institute of Physics, University of Leoben, 8700 Leoben, Austria

In the present study, the growth of thin para-hexaphenyl (6P) films on silicon oxide has been investigated. The 6P layers were fabricated by hot wall epitaxy (HWE) at substrate temperatures between room temperature and 490 K. As substrate, a Si(100) wafer covered with native oxide was used. Conventional tapping mode atomic force microscopy (TM-AFM) revealed islands of upright standing 6P molecules in the sub-monolayer regime. Domains of different molecular orientation could be distinguished by transverse shear force microscopy (TSM). The influence of the growth conditions on the domain size and the influence of the domain orientation on the growth of the successive layers have been evaluated. HWE turned out to be an excellent method to grow an almost closed single 6P layer with large domain sizes. Support by the Austrian Science Fund FWF is acknowledged.

MM 26.74 Tue 14:45 Poster C

Bucky ball island morphologies on CaF_2: Theory and Experiment — •Martin Körner[1,2], Felix Loske[2,3], Mario Einax[1], Angelika Kühnle[3], and Philipp Maass[1,2] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany — [3]Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany

Self-organized growth of C60 molecules deposited on insulator substrates such as $CaF_2(111)$ yield novel types of morphologies: regular triangular double layers as well as strange irregular islands with hexagonal-type shape, double layer rims at the island edges and channels directed towards the interior of the islands. The relative fraction of the two types of morphologies changes with the temperature. We present a theoretical model to predict these morphologies based on a facilitated de-wetting mechanism of C60 molecules in the first layer in the presence of nearby C60 molecules in the second layer. Extensive Kinetic Monte Carlo (KMC) simulations of this model show good agreement with the experimental observations. In particular they support conjectures from experimental findings that the channel structures of the irregular islands form after deposition. The theory moreover provides an explanation for the regular triangular shapes despite absence of epitaxial matching with the substrate lattice. Detailed consideration of the rates for the diffusion and de-wetting processes in connection with scaling arguments allows us to determine effective energy parameters that govern the growth kinetics in this system.

MM 26.75 Tue 14:45 Poster C

Computer tomographic investigation of Ostwald ripening — •Thomas Werz and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Similar to grain growth, Ostwald ripening is a competitive coarsening phenomenon in which larger particles grow at the expense of smaller ones. Improved understanding of Ostwald ripening—in particular, at volume fractions of the coarsening phase above 90%—is crucial to several technological applications, such as aging of multiphase metallic materials and liquid-phase sintering. Although such high volume fractions lie well outside the scope of current analytic modelling, they are feasible to study with modern methods of computer simulation and micro-computed tomography (microCT). Indeed, the latter technique promises to deliver *in situ*, real-time images of Ostwald ripening when carried out with synchrotron radiation. Alternatively, the evolution of sample microstructure can be characterized stepwise by alternating scans in a laboratory microCT at room temperature with *ex situ* anneals to induce coarsening. We have followed such a procedure to obtain 3D datasets of Ostwald ripening as it occurs in semisolid Al-Cu binary alloys. Segmentation of the tomographic reconstructions yields time-dependent maps of particle shapes and sizes that can serve both as starting configurations and as experimental tests for computer simulations of the coarsening process.

MM 26.76 Tue 14:45 Poster C

Is abnormal growth actually the norm in nanocrystalline materials? — •Jules M. Dake, Heiko Paul, and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Nanomaterials may enjoy a privileged place in the fantasies of science-fiction writers, but among researchers studying the phenomenon of grain growth, nanocrystalline specimens suffer from a decidedly dodgy reputation. Not only do they generally contain significant impurity levels (though not necessarily much higher than those of conventional samples, when normalized to the total area of grain boundaries), but experiments designed to pin down characteristic parameters like the growth exponent or activation enthalpy for boundary migration are disappointingly inconsistent. Add to this the suspicion that microstructural entities like triple junctions or quadruple points could modify the kinetics of boundary migration for nanosized grains, and you have a recipe for chaos! To cut through this fog, we carried out a systematic study of isothermal grain growth in nanocrystalline Fe using high-temperature x-ray diffractometry—only to be confronted by indirect evidence for the evolution of grain-size distributions in a manner reminiscent of abnormal grain growth. In order to quantify the microstructural inhomogeneity directly and, thereby, clarify the origins of the x-ray results, we subjected select samples at various stages of annealing to microscopic study using EBSD and TEM. The results indicate that it will not be easy to pin the blame for abnormal growth in nanocrystalline Fe on the usual suspects, like precipitates or texture effects.

MM 26.77 Tue 14:45 Poster C

Segregation stabilization of nanocrystalline binary alloys at low solute concentrations — •Lionel Kroner and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Although enhanced properties are predicted for the nanocrystalline state of many materials, the technological exploitation of such improvements generally requires long-term stability of the microstructure at room temperature and short-term stability during processing (e.g. hot pressing, if highly dense bulk samples must be produced from powders). Therefore, effective strategies must be developed to suppress the strong driving force for grain growth that is always present in nanocrystalline materials owing to the very small average grain size. The deliberate addition of an atomic species that segregates to the grain boundaries has already been shown to impart a dramatic improvement in the thermal stability of nanocrystalline Pd powders alloyed with Zr [1]. Can this approach be extended to other materials systems? To answer this question, we prepared a variety of Ni-based and Fe-based nanocrystalline alloys by ball milling elemental powders with small amounts of Zr, Ti, Mo or Co. The higher the segregation tendency, the stronger we expect the inhibiting effect of the solute species to become on grain growth. Using x-ray diffraction, we tested this hypothesis by examining the thermal stability of the samples as a function of annealing temperature, solute concentration and enthalpy of segregation.

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MM 26.78 Tue 14:45 Poster C

Layer growth of perovskites: computing surface structure and energy barriers as a prerequisite for KMC calculations — •Petar Petrov[1], Hannes Guhl[1,2], and Wolfram Miller[1] — [1]Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin — [2]Fritz-Haber-Institut der Max-Planck Gesellschaft, Faradayweg 4-6, 14195 Berlin

Growing smooth perovskite thin films is the basis of utilizing their promising piezo- and ferroelectric properties in technical applications. In order to understand the deposition processes on atomistic scale kinetic Monte-Carlo (KMC) simulations have been started [1]. However, the activation energies for the relevant surface processes have to be provided by other calculations. The most accurate source are density functional theory calculations, which we have performed for oxygen and hydrogen atoms as well as for water molecules (for oxygen see [2]). On the other hand, the complexity of the problem involving the calculation of many energetic barriers prohibits an in-depth DFT-study of the entire growth process. Therefore, we also use force-field methods based on classical potentials in order to obtain energy barriers for more complex situations within a reasonable time. Potential parameters are adjusted to the results of the DFT calculations and empirical data available in literature.

[1] Petar Petrov, Hannes Guhl and Wolfram Miller, phys. stat. sol. b **245** (2008), 2649

[2] Hannes Guhl, Wolfram Miller and Karsten Reuter, Surf. Sci. (2009) in press

MM 26.79 Tue 14:45 Poster C

Self-organized growth of helicenes on calcite (104) surfaces: Monte Carlo Simulations and Experiments — •Tobias Richter[1], Philipp Rahe[2], Markus Nimmrich[2], Mario Einax[1], Martin Körner[1,3], Angelika Kühnle[2], and Philipp Maass[1,3] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [3]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

Helicene molecules deposited on calcite(104) substrates form one-dimensional double-strands along the [010] direction of the (104) surface. These effectively one-dimensional morphologies show a particular ripening process in the post-nucleation regime due to strong anisotropic diffusion. Kinetic Monte Carlo simulations and extensions of mean-field rate equations are presented to model the increase of the mean chain length of the helicene clusters in dependence of the annealing time. The ripening process exhibits two characteristic time regimes in agreement with the experimental observations.

MM 26.80 Tue 14:45 Poster C

Molecular dynamics simulations of ion transport at the crystal-melt interface during the crystallization of superionic calcium fluoride — •Detlef Stock and Peter Görnert — INNOVENT e.V., Prüssingstr. 27B, D-07745 Jena, Germany

The crystallization of superionic conductors such as calcium fluoride from the melt shows a peculiarity which is due to the liquid-like mobility of anions in the crystalline phase. To understand the atomistic mechanism of the growth process we peform nonequilibrium molecular dynamics (MD) simulations of isothermal crystal growth of calcium fluoride from its undercooled melt for the low index {100}, {110}, and {111} crystal-melt interfaces. The MD simulations are based on parameterized potentials describing long-range Coulomb and pairwise short range interactions. We investigate the ion transport at the interface in terms of ion mobility and average coordination number of the ions as a function of the distance to the interface. As a result we observe the freezing of the cation sublattice, whereas there is only a slight decrease of the anion mobility in the growing crystal. Finally, a comparison of the growth kinetics of superionic calcium fluoride with results for simple fcc metals will be given.

MM 26.81 Tue 14:45 Poster C

Numerical studies on grain growth of Si: Influence of surface energy anisotropy — •Giordano Cantù and Wolfram Miller — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin

With the developing market for multi-crystalline Si dedicated for photovoltaic applications the interest in understanding the details of the grain growth has increased. First numerical simulations on grain growth of Si have been performed by I. Steinbach [1] and detailed experimental investigations have been performed in the group of K. Nakajima (e.g. [2]). Corresponding (2D) calculations to one of the experiments have been performed by Chen *et al.* using a four-fold anisotropy with an anisotropy of 25% [3]. We have performed 2D computations of grain growth into an undercooled using the phase-field model of Warren *et al.* [4] and different approaches for the anisotropy of the surface energy. The influence of the dependence of the surface stiffness as a function of the crystal orientation on the growth kinetics is discussed.

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MM 26.82 Tue 14:45 Poster C

Morphology of Graphene Layers on Ir(111) Studied by SPA-LEED — •Dennis Meyer, Hichem Hattab, Giriraj Jnawali, Dirk Wall, Frank-Joachim Meyer zu Heringdorf, and Michael Horn-von Hoegen — Fakultät für Physik und Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany

We used SPA-LEED to investigate the morphology of graphene layers on Ir(111) at different growth temperatures. The decomposition of ethylene at 1040°C results in a highly oriented graphene layer. The LEED pattern solely shows the moiré spots surrounding each Ir(111) integer order spot. These satellites arise from the 10% mismatch between the two hexagonal lattices. Between 600°C and 1000°C we observe in addition a broad distribution of almost randomly oriented graphene domains which cover the majority of the surface. These domains give rise to broad arcs in the LEED pattern. There is no commensurate order with respect to the Ir(111) substrate. Another minority graphene domain is rotated by 30° with respect to the Ir(111) lattice, locks in in registry with the substrate, and gives rise to a sharp spot between the moiré patterns of the ordered phase.