MM 17: Poster Session

Time: Monday 17:00–19:00 Location: Poster B

MM 17.1 Mon 17:00 Poster B

Oxidation of monovacancies in graphene by oxygen molecules — Thaneshwor Kaloni, Yingchun Cheng, and •Udo Schwingenschlogl — 4700 King Abdullah University of Science and Technology Thuwal 23955-6900

We study the oxidation of monovacancies in graphene by oxygen molecules using first principles calculations. In particular, we address the local magnetic moments which develop at monovacancies and show that they remain intact when a molecule is adsorbed such that the dangling carbon bonds are not fully saturated. The observed value of magnetic moment is 1.35 Bohr Magneton for monovacancy and it becomes 1.86 Bohr Magneton by oxygen adsorption on monovacancy in graphene. However, the lowest energy configuration does not maintain dangling bonds and is found to be semiconducting. Our data can explain the experimentally observed behavior of graphene under exposure to an oxygen plasma.

MM 17.2 Mon 17:00 Poster B

Thermal stability and crystallization of magnetron sputtered amorphous Si2C — •René Gustus[1,2], Wolfgang Gruber[2], Lienhard Wegewitz[1,3], Harald Schmidt[2,3], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Straße 42, Clausthal-Zellerfeld, Germany — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

During the last decades, amorphous silicon carbide (SiC) has attracted much attention in several fields of scientific research. Non-stoichiometric amorphous SiC became of specific interest due to the possibility of tailoring the material properties by varying its chemical composition. We investigated the thermal stability and the crystallization of magnetron sputtered amorphous non-stoichiometric Si2C deposited on silicon substrates, by means of XPS, AES, XRD, AFM and SEM. Crystallization of amorphous Si2C takes place at temperatures around 800 °C, accompanied by the growth of silicon crystalls on the surface. Annealing at 1200 °C for 2 hours leads to crystallization of silicon and silicon carbide, coupled with the formation of large structures and a silicon enrichment in the surface region of the film. After 20 hours of anealing at 1200 °C, the crystalized silicon has disappeared from the surface and no silicon enrichment is detectable any longer. The experimental results and the underlying processes are discussed.

MM 17.3 Mon 17:00 Poster B

Atomistic study of the elastic properties of alpha' martensite crystals — •Nina Gunkelmann and Herbert M. Urbassek — Fachbereich Physik und Forschungszentrum OPTIMAS, Universität Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern

Material phycisists have long-standing experience in modeling of pure iron by atomistic simulations. There exist a number of interaction potentials describing the properties of this material. In contrast, only a few interatomic potentials have been developed for the iron-carbon system; these have not yet been fully characterized with respect to the mechanical properties of martensitic crystallites. This seems surprising because of the high-technologic importance of steel. In this work the elastic properties of iron-carbon crystals are characterized using molecular dynamics simulation and compared with available experimental data.

MM 17.4 Mon 17:00 Poster B

Measurement of nucleation rates using fast scanning calorimetry on samples prepared by the Droplet Emulsion Technique (DET) — •Christian Simon, Joachim Bokeloh, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

The most difficult part in heterogenous nucleation experiments is the control of the heterogenous nucleant. On one hand, parasitic nucleants like the container wall and impurities must be removed, and on the other hand the target nucleant phase must be kept at a constant potency. The DET is uniquely suited to accomplish this task. With the DET microsized droplets of a material are prepared by heating it above the melting temperature in a special organic solution and then dispersing it to a fine emulsion of droplets by violent stirring. While the fine dispersion reduces the influence of impurities, the organic solution forms a non-catalytic surface layer and thus reduces the nucleation potency of the surface.

The nucleation rate is evaluated by a statistical analyses that treats nucleation as a non-homogenous Poisson process. A DSC measurement is used to analyse the undercooling of an ensemble of droplets. A fast scanning nano-calorimeter (10 K/s - 100000 K/s) is used to analyse the undercooling and nucleation rate over a large number of repeated heating-cooling-cycles on single droplets, allowing for an heretofore unprecedented accuracy in the nucleation rate measurement.

MM 17.5 Mon 17:00 Poster B

New deposition concept for the precise tailoring of nanocomposites with a gas aggregation cluster source — •Björn Gojdka[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Viktor Hrkac[2], Jian Xiong[1], Lorenz Kienle[2], and Franz Faupel[1] — [1]Institute for Materials Science (Multicomponent Materials), Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstraße 2, D-24143 Kiel, Germany — [2]Institute for Materials Science (Synthesis and Real structure), Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstraße 2, D-24143 Kiel, Germany

Nanocomposites with embedded magnetic particles are of special interest due to their unique properties which are, for example, highly relevant for data storage or high-frequency applications. However, in order to tailor a nanocomposite for a certain application, advanced process control is necessary. In addition, during deposition most magnetic materials react with a non-inert process atmosphere or the matrix constituents, thus degrading the ferromagnetic properties of the nanoparticles in the composite. We present a new concept for the precise tailoring of a wide variety of nanogranular composites based on a modified co-sputtering concept with a gas aggregation cluster source. To demonstrate the feasibility of the concept, magnetic cobalt nanoparticles are embedded in a dielectric matrix. Subsequently, the chemical, magnetic and structural properties of the composite were investigated by energy dispersive x-ray spectroscopy, vibrating sample magnetometry and transmission electron microscopy.

MM 17.6 Mon 17:00 Poster B

Nonlinear response of metallic glasses at high applied stresses and nonlinear effects of damping behaviour below to above the glass transition temperature — •Antje Krüger, Moritz Schwabe, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The α- and β-processes in metallic glasses can be described within the model of the potential energy landscape (PEL). These processes illustrate barriers for a change of local configurations and can be varied by external stresses. When applying a constant stress the sample responds in a combination of different behaviours, elastic, anelastic and plastic.

In the previous work we studied the anelastic contribution in order to obtain information about the damping behaviour. The results showed an exponential correlation to temperature and stress [1]. Now, we also can estimate the activation volume of the α- as well as the β-process using these creep-recovery-methods [2]. Furthermore we investigate in the viscous flow the Newtonian and non-Newtonian behaviour when increasing the elastic strain σ_0/E. This can be compared to well known results in polymers, granular and colloidal systems. Work supported by FOR1394 and GRK782.

[1] M. Schwabe, D. Bedorf and K. Samwer, The European Physical Journal E (2011), 34, 91

[2] M. Schwabe, S. Küchemann, H. Wagner, D. Bedorf and K. Samwer, Journal of Non-Crystalline Solids (2010), 357, 490-493

MM 17.7 Mon 17:00 Poster B

Ab-Initio Hamiltonian and Hedin's Equations for Phonon-Induced Effective Electron-Electron Interaction — •Ronald Starke — Department of Computational Materials Physics, Uni Wien, Sensengasse 8/12, A-1090 Wien, Austria

Ab-initio methods are usually applied to electronic structure theory with an electron-electron interaction given by the Coulomb potential.

Nonetheless, it is well-known that the nuclear degrees of freedom (regrouped as phonons) lead to a broad range of effects from modifications in the optical spectra up to superconductivity. On a fundamental level, the phononic degrees of freedom constitute a physical system in its own right. Hence, the total system cannot be described by a purely electronic Hamiltonian. As a first approximation, one disregards the phononic degrees of freedom by taking them into account through an effective electron-electron interaction. This gives rise to a huge field of effective models, the most prominent being BCS theory. However, these effective models clearly do not match the standards of ab-initio electronic structure calculations: not only is the effective phonon-induced electron-electron interaction not parameter free, even worse, important ingredients of the fundamental ab-initio electronic Hamiltonian like the Coulomb potential are not taken into account. We review how this problem can be overcome by the addition of an phonon induced effective but ab-initio electron-electron interaction to the standard ab-initio Hamiltonian and discuss the corresponding modified Hedin equations.

MM 17.8 Mon 17:00 Poster B

Diffusion and microhardness in ultrafine grained nickel — •Simon Trubel, Sergiy Divinski, Gerrit Reglitz, Jörn Leuthold, and Gerhard Wilde — Westfälische Wilhelms-Universität, Institut für Matrialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

Ultrafine grained and nanocrystalline materials produced by methods of severe plastic deformation have roused a growing interest in science and technology. To determine how certain characteristics of internal interfaces in a material are affected by severe deformation, diffusion is a suitable method. The material under investigation is nickel in a purity of 99.6%. High pressure torsion (HPT) is applied where nickel discs are subjected to quasi-hydrostatic pressure of 2 GPa and torsionally deformed several times. Ultrafine grained Ni is produced and grain boundary self-diffusion is measured at several temperatures applying the radioactive isotope 63Ni. The HPT process refines the grain size in the material and the grain boundary diffusion is significantly enhanced. Nanoindentation is used to obtain information about mechanical properties of the material and their evolution with annealing temperature.

MM 17.9 Mon 17:00 Poster B

From structure refinements of ε-Al–Pd–Mn phases toward decagonal quasicrystals — •Benjamin Frigan[1], Marek Mihalkovič[2], and Hans-Rainer Trebin[1] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

We have studied and resolved occupancy correlations in the existing average structure model of the complex metallic alloy ξ'-Al–Pd–Mn, which has approximately 320 atoms in the unit cell and many fractionally occupied sites. Model variants were constructed systematically in a *tiling-decoration approach* and subjected to simulated annealing by use of both density functional theory and molecular dynamics with empirical potentials.

The main structural building blocks of ξ' are pseudo-Mackay icosahedral (PMI) clusters which form columns parallel to (0,1,0) and when projected are vertices of a hexagonal tiling. The tiling representation allows to extend structure models for the ξ'-phase to structure models of other closely related phases where the projections of the PMI columns also form pentagon and nonagon tiles. Our refined tiling-decoration model applies to any structure within the so-called ε-phases family.

We further extend our tiling-decoration model and present a detailed atomistic description of all tiles that are observed in the decagonal quasicrystalline phase. We show how aspects of both the ε-phases and the decagonal phase can serve as a starting point for an accurate microscopic modeling of the *metadislocations*.

MM 17.10 Mon 17:00 Poster B

Investigation of stable intermediate states in fourfold nanosystems — •Andrea Ehrmann[1] and Tomasz Blachowicz[2] — [1]Hochschule Niederrhein, Faculty of Textile and Clothing Technology, Mönchengladbach, Germany — [2]Institute of Physics, Silesian University of Technology, Gliwice, Poland

In systems of four crossed ferromagnetic nano-wires, pronounced magnetization steps in the hysteresis loops have been found using micromagnetic simulations [1]. The steps can be attributed to stable intermediate states, similar to flux-closed vortex states in ferromagnetic nano-rings.

Due to the fourfold anisotropy of the system of four coupled nanowires, these states can be distinguished even by measuring the magnetization of the whole system, giving rise to four separated states in the absence of an external magnetic field. Opposite to actual trials with nano-rings or layered structures, no additional method of symmetry breaking is necessary. Downscaling the system leads to qualitative changes in the magnetization reversal, which have to be taken into account by changing the material or adjusting the design.

Such a system can be utilized, e.g., in quaternary (four states, i.e. two bits per magnetic nano-object) magnetic storage applications.

[1] T. Blachowicz, A. Ehrmann: Fourfold nanosystems for quaternary storage devices, J. Appl. Phys. 110, 073911 (2011)

MM 17.11 Mon 17:00 Poster B

Design and Operation of a Nano-Calorimeter for high Sensitive and Fast heating rates measurements — •Mostafa Mohamed, Joachim Bokeloh, Tae-Eun Song, and Gerhard Wilde — Institute of Materials Physics, Westfalische Wilhelms University Muenster,Muenster,48148,Germany

A thin-film differential scanning calorimetric (TDSC) technique has been developed based on Silicon-Nitride (Si-Nx) membranes, for use as a Nano-calorimeter detector in high-sensitivity measurements. The Nano-calorimeter is specifically designed to determine the thermal properties and heat capacity of nano-structured materials, with very high sensitivity values and fast heating rates (104 K/S). The (Si-Nx) membrane was used as a low thermal mass mechanical support structure. The measurements of the system are accomplished via electrodes of Pt or Au that are used for resistive heating and resistive temperature measurement simultaneously. The method shall be applied first to measure the melting of various amounts of pure evaporated metal thin films.

MM 17.12 Mon 17:00 Poster B

Direct Single Electron Imaging with a pnCCD for TEM — •Henning Ryll — PNSensor GmbH, München

Promising better resolution and sensitivity, work on a spatially resolving direct electron detector, based on a pnCCD is presented.

A pnCCD is a back-illuminated silicon detector, which is sidewards depleted. By applying appropriate voltages to both sides, the whole 450 um thick bulk, high-purity n-type silicon is depleted.

Up to 1000 full frames per second are achieved, enabling the imaging of single electrons in ultra-low dose modes and the observation of changes in samples. Each electron creates a signal easily distinguished from the noise. The final image is obtained by successive addition of individual frames and their intensities. Additionally image processing at the single incident electron level and its signal can be performed.

In order to determine the characteristics of the pnCCD, one type with a pixelsize of 51x51um^2 was tested on a Phillips CM12 120 keV TEM. A slanted knife edge was placed in front of the detector to determine the MTF. Operating at 120 keV and a low dose, applying signal processing allowed for a software subpixel resolution, improving the MTF to >40% @ Nyquist.

Simulations complementing the experimental data will be presented, as well as the expected pixel patterns and their analysis for different energies.

MM 17.13 Mon 17:00 Poster B

Investigation of strain fields along shear bands in a deformed Pd40Ni40P20 bulk metallic glass — •Severin Schlottbom, Jonas Bünz, Jörn Leuthold, Stefan Ostendorp, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Plastic deformation of metallic glasses induces shear bands, which form quasi-instantaneously once a critical loading is exceeded. The mechanism of deformation is essential for the mechanical properties of amorphous metals, but not deeply understood yet. The knowledge of strain fields along a single shear band might provide access to understanding the basic deformation mechanism of the shear transformation zones (STZ) forming the shear bands. In this work the initiation of shear bands and their influences on the adjacent unaltered matrix is investigated. Undeformed Pd40Ni40P20 bulk metallic glass was coated with gold nanodots by PVD, delivering a nanoscale grid, which is used to monitor the strain fields during shear deformation. The as-cast and subsequently cold-rolled samples were examined by scanning electron microscopy and digital image correlation is used in order to determine the strain fields.

MM 17.14 Mon 17:00 Poster B

Generation of force field for molecular dynamic simulations of zirconia — •Andreas Irmler, Philipp Beck, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik (ITAP) , Universität Stuttgart

We have generated force fields for crystalline and molten metal oxides. With these force fields, we intend to simulate microstructural and thermodynamic properties of systems with millions of atoms. We use DFT calculations to obtain forces, stresses and energies of reference systems with several hundred particles. Via potfit [1], a force matching package, we generate interaction potentials by adjusting its parameters to optimally reproduce the reference data computed in ab-initio calculations. We use Wolf summation [2] to handle long range electrostatic interactions. This direct, pairwise summation method scales linearly in the number of particles. The polarizability of oxygen atoms is described with Tangney-Scandalo [3] force field model. With this approach we have created force fields for several metal oxide systems in liquid and solid state. These force fields were tested in molecular dynamic simulations and show good agreement with experimental results. In the present contribution, we show the application to crystalline zirconia.

[1] P.Brommer *et al.*, Modelling Simul.Mater.Sci.Eng. **15** ,295 (2007).
[2] D. Wolf *et al.*, J. Chem. Phys. **110**, 8254 (1999).
[3] P. Tangney and S. Scandalo, J. Chem. Phys. **117** 8898 (2002).

MM 17.15 Mon 17:00 Poster B

Order-disorder transformation in copper-gold alloys revisited by in situ X-ray diffraction — •Max Metelmann, Martin Peterlechner, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institute of Materials Physics, Wilhelm-Klemmstr. 10, 48149 Münster, Germany

CuAu alloys with an equi-atomic composition exhibit a well known order-disorder phase transformation in the solid state. Detailed analyses of this order-disorder transition were performed using in situ heating X-ray diffraction.This method enables temperature and time-resolved studies of the long range order parameter, which can be calculated from diffraction spectra. By means of in-situ X-ray diffraction, the temperature dependence of the peak intensity has been investigated, i.e. the Debye-Waller factor has been determined. In addition, the decrease of the peak intensity with increasing temperature and increasing angle of incidence is modeled. The comparison between experiments and calculations indicates that the experimental results are imprecisely described. The results are discussed with respect of corrections to the theoretical description of the Debye-Waller factor.

MM 17.16 Mon 17:00 Poster B

Finite element based fatigue predictions for Thermal-Acoustical-Protective-Shields — •Martin Kollenrott and Othmar Marti — Department of Experimental Physics, Ulm University

In the engine compartment more and more temperature-sensitive parts are being used. Thermal-Acoustical-Protective-Shields (TAPS) protect these parts from high temperature impact. TAPS are exposed to different periodic forces and temperatures mainly induced by the engine. The subject is to guaranty the lifetime resistance against fatigue of the part. In the ongoing project a finite element based model for fatigue of TAPS has to be developed.

To predict durability, dynamic and forming stresses are important. For a dynamic stress prediction it is necessary to determine loss factors for the 3-D formed thin sheet metal layers. These measurements are performed with a laser-vibrometer with impulsive or vibratory excitation of the parts. To determine forming stresses, finite element based forming simulations are performed. A Woehler curve depending on the pre-stressed material at the previous forming process is used for every node in the finite element mesh to predict cracks.

MM 17.17 Mon 17:00 Poster B

Ab initio and kinetic Monte Carlo modelling of Fe-Cu-Ni-Mn alloys — •Stephen Hocker, Peter Binkele, Alejandro Mora, and Siegfried Schmauder — Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Universität Stuttgart

Formation and growth of precipitates in thermally aged Fe-Cu-Ni-Mn alloys at temperatures above 573 K is investigated by kinetic Monte Carlo simulations. A thermally activated vacancy diffusion mechanism on a rigid bcc lattice is used to characterize the processes of nucleation and growth of Cu clusters. Important input parameters for the Monte Carlo simulations are mixing energies and vacancy formation energies. DFT based ab initio calculations are presented which provide these data. Monte Carlo simulations are performed with a thermodynamically based set of input parameters as well as with the ab initio based set of parameters. It is shown that the Monte Carlo results are very sensible regarding these input data. The influence of the Ni and Mn atoms in the precipitation of Cu rich clusters is analyzed for both simulation setups.

MM 17.18 Mon 17:00 Poster B

Synthesis and electrochemical properties of tailored $LiMPO_4$ (M= Mn, Co) — •Christoph Neef, Carsten Jähne, and Rüdiger Klingeler — Kirchhoff Institut für Physik, Universität Heidelberg, Germany

Due to their high stability and theoretical capacity, transition-metal olivine phosphates offer a large potential for application as positive electrodes in Li-Ion batteries. Among $LiFePO_4$, which is already used in high power cells, $LiMnPO_4$ and $LiCoPO_4$ are interesting compounds because of their high open cell voltage vs. Lithium of 3.9V and 4.6V respectively. Here we report on the microwave assisted hydrothermal synthesis of $LiMnPO_4$ and $LiCoPO_4$ and their electrochemical characterisation by means of cyclic voltammetry and impedance spectroscopy. Variation of synthesis parameters as well as wet ball milling are used for size and shape tayloring of the particles. PEIS is used to study the morphology influence on high and low frequency impedance and thus on charge transfer resistances, ion diffusion and double layer capacitances. We found that size reduction of particles increases the electrochemical performance, however the extensive application of ball milling may cause a loss of crystal structure and thus reduces the ability of lithium intercalation / deintercalation.

MM 17.19 Mon 17:00 Poster B

Phason flips in quasicrystals: Interpretation of HRTEM data using kinetic Monte Carlo simulations — •Hansjörg Lipp and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

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

On the one hand, we analyze the temporal evolution and statistical properties of the spots shown on HRTEM images provided by K. Edagawa. On the other hand, we perform kinetic Monte Carlo simulations [2], using several statistical model systems, e.g. based on a structure model for d-Al-Cu-Co suggested by Zeger et al. [3]. There rings of ten atoms can perform flips by collective motion of atoms inside decagonal double layers.

We relate the experimental data to our simulation results, and demonstrate how flip frequencies depend on the number of decagonal layers and on the strength of their interaction.

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

MM 17.20 Mon 17:00 Poster B

Atomistic simulation of severe plastic deformation-induced "high-energy" state of grain boundaries — •Lisa Neier[1], Sergiy Divinsky[1], Anatha Padmanabhan[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Münster — [2]University of Hyderabad, India

A comparison of microstructures, properties and transport kinetics in materials subjected to the last stages of severe plastic deformation (SPD) or steady-state superplastic flow indicates a number of unexpected similarities especially with respect to the interface response on the deformation, such as formation of an interface hierarchy, deformation localization, grain boundary sliding events when dislocation activities are suppressed, etc. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle grain boundaries in SPD-processed materials in terms of the concept of shear localization in the interfaces and choosing oblate spheroids as basic units of sliding.

"Non-equilibrium" grain boundaries in Cu are simulated. The individual simulation steps include generation of a grain boundary; determination of regions corresponding to the oblate spheroids on the

boundary plane; introduction of an extra free volume (a fraction of atoms in the oblate spheroids is simply deleted) and shearing of the oblate spheroids by a given amount. By energy minimization, a high-energy state of the grain boundary is found which corresponds to about 4% additional free volume and 0.1 unit shear. The subsequent response of such an interface on the applied shear is analyzed.

MM 17.21 Mon 17:00 Poster B

Towards kinetic Monte-Carlo simulations with ab initio accuracy — •Martin Leitner[1], Tobias C. Kerscher[1,2], Stefan Müller[2], and Raimund Podloucky[1] — [1]University of Vienna, Institute of Physical Chemistry, Vienna, Austria — [2]Hamburg University of Technology, Institute of Advanced Ceramics, Hamburg, Germany

For the Ni–Al and Fe–Al alloy system we present the first steps towards kinetic Monte-Carlo (KMC) simulations with ab initio accuracy. Many body interactions which describe the energetics of both the local minima and migration states are included by cluster expansions (CE) in the framework of the UNCLE code [1].

In this model approach single atoms jump to vacant nearest-neighbor sites and have to overcome configuration dependent migration barriers. According to transition state theory (TST) jump rates are then derived by the energy difference between initial and saddle point state. The KMC simulations require a) vacant lattice sites, which enforce a ternary CE for a binary compound, and b) the configuration dependent height of the saddle points, which have to be calculated and included in the CE.

We discuss different aspects of jump profiles in the respective systems computed by density functional theory (DFT) calculations.
The support of FWF project 4110 (ViCoM) is acknowledged.
[1] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

MM 17.22 Mon 17:00 Poster B

Interactions in Fe-Pd — •Cédric Sax and Bernd Schönfeld — LMPT, Department of Materials, ETH Zurich

X-ray diffuse scattering was measured from single-crystalline Fe-80 at.% Pd. A state of thermal equilibrium - corresponding to 1073 K - was investigated at room temperature. Maxima of diffuse scattering were found at X positions. Short-range order scattering was separated by the Georgopoulos-Cohen technique and effective pair interaction (EPI) parameters were determined by the inverse Monte Carlo method. In contrast to the set of EPI parameters that were obtained by Mehaddene et al. for Fe-50 at.% Pd, a dominant and positive value for the nearest-neighbor interaction is now found. This outcome indicates a stronger ordering tendency for Fe-Pd with a higher Pd fraction. Using linear interpolation between the EPI parameters at both compositions, shifts in the highest order-disorder transition temperatures of the $L1_0$ and $L1_2$ phases away from stoichiometry are obtained. Direct experiments confirm these findings.

MM 17.23 Mon 17:00 Poster B

Structure and thermal stability of severely plastically deformed Cu84Al16 — •Nazar Ibrahim, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-University Münster,Germany

Severe plastic deformation (SPD) can produce ultrafine grained materials with extraordinary mechanical properties. High strength and relatively good ductility are attributed to their fine microstructure. In this work, structure modification by high pressure torsion (HPT) and the thermal stability of the resulting microstructure are investigated for the Cu*16 at.% Al alloy. For this alloy, a propensity for the formation of five-fold twinning has recently been reported. Disks of thickness of 0.8 mm and diameter of 10 mm were processed via HPT for five revolutions at room temperature using an imposed pressure of 6.0 GPa and rotational speed of 1 rpm. Structural and thermal analysis were carried out using X-ray diffraction, transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). The DSC experiments using constant heating rates showed two exothermic peaks in the temperature range from 30°C to 450°C. After HPT a highly distorted structure was observed, including dislocations, fragmented grains and twins. The twin thickness in Cu84Al16 has been determined from TEM observation to be in the range of 2 to 6 nm. These small thicknesses are in agreement with the low stacking fault energy of the alloy. The results are discussed with respect of the reported five-fold twinning in this alloy.

MM 17.24 Mon 17:00 Poster B

Tuning of the silver ion release from polymer-metal nanocomposites containing gold-silver alloy or gold-core/silver-shell nanoparticles — •Nisreen Alissawi, Irmak Kocabas, Vladimir Zaporojtchenko, Thomas Strunskus, and Franz Faupel — Institute for Materials Science - Multicomponent Materials, Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiser Str. 2, 24143, Kiel, Germany

The tuning of silver ion release could be important for antimicrobial applications of silver where a controlled release is desired to prevent e.g. damage of human cells. Two dimensional Au-Ag alloy or Au-core/Ag-shell nanoparticle ensembles with various compositions on PTFE were prepared by physical vapor deposition (PVD) techniques and silver ion release kinetics in water were studied by determination of the dissolved silver using atomic absorption spectroscopy (AAS). Changes in the morphology, optical properties and composition of the nanocomposites were examined by using transmission electron microscopy (TEM), UV-visible spectroscopy (UV-Vis) and X-ray photoelectron spectroscopy (XPS), respectively. Results indicate that with increasing the gold fraction in the Au-Ag alloy nanoparticles a strong improvement of the oxidation resistance of the AgNPs occurs. This can be a good way to control the release of silver ions in solutions. Moreover, the effect of a polymer barrier of certain thickness was investigated for both model systems and the silver ion release rate was slowed down.

MM 17.25 Mon 17:00 Poster B

Cooling rate dependence of undercooling of pure Sn single partially molten drop by fast scanning calorimetry — •Bin Yang[1], Alexander Sasha Abyzov[2], Evgeny Zhuravlev[1], Yulai Gao[3], Jürn W. P. Schmelzer[1], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]National Science Center, Kharkov Institute of Physics and Technology, 61108 Kharkov, Ukraine — [3]Shanghai Key Laboratory of Modern Metallurgy & Materials Processing, Shanghai University, Shanghai 200072, P.R. China

The partial melting of a pure Sn single micron sized particle is successfully performed by non-adiabatic differential fast scanning calorimetry. In a large range of cooling rates spanning three orders of magnitude solidification undercooling is observed for the partially molten particle. The cooling rate dependence of undercooling is correspondingly investigated. Our data indicate that the kinetics of nucleation changes with decreasing cooling rate. The differential fast scanning calorimetry opens up the possibility to experimentally study the kinetics of nucleation and growth processes of single metallic particles at rapid solidification extending the theoretical analysis of these processes performed in previous studies.

MM 17.26 Mon 17:00 Poster B

Texture gradient in ultrafine-grained Ti/Al composite wires produced by accumulative swaging and bundling — •Andy Eschke[1], Juliane Scharnweber[1], Carl-Georg Oertel[1], Tom Marr[1,2], Jan Romberg[1,2], Jens Freudenberger[2,3], Uta Kühn[2], Ludwig Schultz[1,2], Jürgen Eckert[1,2], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, Germany — [2]Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [3]Institut für Werkstoffwissenschaft, TU Bergakademie Freiberg, Germany

Various top-down processes of severe plastic deformation (SPD) like equal channel angular pressing, high pressure torsion or accumulative roll bonding are well known for producing ultrafine-grained (ufg) microstructures. The evolution of texture with respect to deformation by an alternative SPD process, called accumulative swaging and bundling (ASB), is shown for ufg Ti/Al wires, suitable for structural materials because of their high specific strength. An Al rod was stacked into a Ti tube and swaged with an area reduction of approximately 20% per pass to a logarithmic strain of 4.3. The resulting composite wire was cleaned, cut into 37 pieces, stacked into a Ti tube (of initial dimension) in a hexagonal arrangement and then swaged again. This procedure can be repeated arbitrarily. The texture gradient of the ASB composites was studied using a X-ray micro diffraction system D8 DISCOVER (Bruker AXS GmbH) equipped with a micro focus X-ray tube IμS and an area detector Vantec-2000. The results will be discussed with respect to processing and grain refinement.

MM 17.27 Mon 17:00 Poster B

Phase Field Simulations of Martensitic Transformation in Thin Films — •Alexander Auge, Niclas Teichert, and Andreas Hütten — Bielefeld University, Department of Physics, Uni-

versitätsstr. 25, 33615 Bielefeld, Germany

Magnetic shape memory materials like Ni-Mn-Ga and Ni-Mn-Sn have been intensively investigated in the past few years due to their potential applications in magnetic cooling or actuators. The physical origin of these effects is the martensitic transformation (MT) in combination with ferromagnetism. For many applications, like magnetic cooling, thin films are advantageous or even mandatory. The confinement due to the film thickness and also the constraint of the substrate can have a major influence on the transition and even hinder a MT completely. To understand what the major contributions to the change in the MT are and how to optimize the performance of the MT in thin films, phase field simulations are carried out. A three dimensional Landau theory for multivariant phase transformations developed by Levitas et al. [1] is used in the framework of finite element simulations. The most relevant energy contributions in dependence of film thickness and the resulting microstructure are presented.

[1] V. I. Levitas and D. L. Preston, Phys. Rev. B 66, 134207 (2002)

MM 17.28 Mon 17:00 Poster B

X-ray diffraction studies on low alloyed and high-Mn steels with TRansformation and TWinning Induced Plasticity (TRIP, TWIP) — •Andre Steffen[1], Hendrik Quade[2], Raphael Twardowski[2], Sascha Buthmann[2], Michael Paulus[1], Christian Sternemann[1], Ulrich Prahl[2], Wolfgang Bleck[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, D-44221 Dortmund. — [2]Institut für Eisenhüttenkunde, RWTH Aachen, D-52072 Aachen.

High manganese austenitic steels and low alloyed TRIP steels combine high strength and formability. Therefore they get high attention regarding the applications in automotive parts and safety-sensitive areas. The excellent mechanical properties of these steels result from different deformation mechanisms, such as the martensitic transformation and twinning. The TRIP and TWIP effect does not only result in an increase in hardening but also postpones necking or damage to later deformation degrees, which leads to a better formability. For the investigation of the TRansformation Induced Plasticity effect during straining several commercial low-alloyed TRIP steels were analysed. The investigations were carried out in-situ using a tensile testing machine. Further investigations on high-Mn steel tensile TWIP samples with varying microstructure were performed. The microstructure was set by annealing and quenching. Afterwards the samples were prestrained to 5 %, 10 %, 20 %, 30 % and 40 % of true strain. The tensile tests were carried out for a temperature range of 123 K to 423 K and a strain rate of 0,004 s^{-1}.

MM 17.29 Mon 17:00 Poster B

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

Lithium titanate (LTO) is used as an anode material in lithium ion batteries, as it reveals both, electronic as well as Li-ion conductivity. Both conductivities and the capability to reversibly intercalate/deintercalate lithium, strongly depends on the lithium diffusivity of the material, which is difficult to obtain in case of powder material, because of its porous structure. Therefore, due to their well defined structure and the absence of e.g. conductive binder, ion-beam sputtered thin film electrodes of LTO are appropriate for diffusion studies, as they give access to the diffusivity of lithium in pure LTO. In this work we prepared thin films of LTO by reactive rf-ion beam sputtering and carefully proofed the structure of the films by X-ray diffraction and transmission electron microscopy. Afterwards, we applied galvanostatic intermittent titration technique (GITT) technique to determine the chemical diffusion coefficient, i.e. by evaluating the electrical potential of the LTO layer vs. lithium, when applying a pulsed current signal. Due to the thin film geometry of our samples, it was possible to reliably evaluate the GITT results by assuming the thin approach and to obtain the lithium diffusivity in LTO as a function of the lithium concentration.

MM 17.30 Mon 17:00 Poster B

Electrochemical tuning of the electrical resistance of nanoporous platinum produced by dealloying — •Eva-Maria Steyskal[1], Maximilian Besenhard[1], Thomas Traussnig[1], Jörg Weissmüller[2], Stephan Landgraf[3], and Roland Würschum[1] — [1]Inst. f. Materialphysik, TU Graz, Graz, Austria — [2]Inst. f. Werkstoffphysik u. Werkstofftechnologie, TU Hamburg-Harburg, Hamburg, Germany — [3]Inst. f. Physikalische u. Theoretische Chemie, TU Graz, Graz, Austria

Nanostructured materials can exhibit electrochemically tunable properties due to their high surface-to-volume ratio. Based on this concept, reversible tunig of mechanical, electrical, and magnetic properties has been demonstrated recently. The present work studies the tunability of the electrical resistance of nanoporous platinum, produced by dealloying of a $Cu_{75}Pt_{25}$ alloy. In the investigated potential range, the charge coefficient $(\Delta R/R_0)/\Delta Q$ exhibits a sign inversion, thus differing from previous results on nanocrystalline, compacted platinum powder [1] as well as nanoporous gold [2]. The resistance behavior in the two charge-coefficient-regimes is attributed to variations in the charge carrier density and interfacial scattering in the positive, as well as the oxygen coverage in the negative sign region. Financial support by the FWF Austrian Science Fund is appreciated (project S10405-N16).

[1] M. Sagmeister et al., Phys. Rev. Lett. **96**, 156601 (2006)
[2] P. Wahl et al., J. Appl. Phys. **108**, 073706 (2010)

MM 17.31 Mon 17:00 Poster B

Atom probe specimen preparation from nanoporous materials — •Björn Pfeiffer, Torben Erichsen, Eike Epler, and Carsten Nowak — Georg-August-Universität Göttingen, Institut für Materialphysik

During the last years open-celled nanoporous foams attracted a lot of attention because of their physical properties and possible technical applications. For example, with their large surface to volume ratio they are ideal for application as catalysts and as electrodes in batteries. To determine the chemical composition of such heterogeneous materials in three dimensions with sub-nanometer resolution atom probe (AP) exactly fits the requirements. However, problems with mechanical stability during analysis and with data reconstruction arise when analyzing non-compact materials. Here, we demonstrate that electron-beam induced CVD is a promising approach to overcome these problems.

For the experiments, nanoporous gold (np-Au) was used as a model system for nanoporous materials. Electron beam induced CVD of organometallic precursors allows to fill the pores of the material in volumes large enough for AP sample preparation with residual voids in the low nanometer range. Fieldevaporation series in FIM with intermediate TEM-imaging reveal that controlled fieldevaporation of both, np-Au and the deposited precursor is possible and that samples are mechanically stable under electric fields necessary for FIM-imaging. The presented results give an outlook on the opportunities given by this method to analyze open-celled nanoporous materials with FIM and AP.

MM 17.32 Mon 17:00 Poster B

Structural aspects of hydride formation in Gd thin films — •Sara Wanjelik, Volkmar Hess, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

Hydrogen in metals has attracted a lot of attention in the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamentel point of view.

For our research we use Gadolinium grown on a W(110) crystal. Depending on the preparation conditions smooth films or islands can be obtained. The investigations were performed with a scanning tunneling microscope. It can also be used in the spectroscopic mode. This allows us to correlate hydrogen-induced electronic and topographic changes on the atomic scale. Offering high amounts of hydrogen to Gd thin films results in the formation of hydrides which exhibit a significantly enhanced lattice volume. Thus, structural changes occur in order to reduce the stress. As a result the surface shows different types of morphological variations. These changes are studied as a function of film thickness.

MM 17.33 Mon 17:00 Poster B

Lithium Iron Phosphate as thin film cathode and in all solid-state batteries — •Mathias Köhler, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Lithium Iron Phosphate (LFP) is widely used as a cathode material in conventional lithium ion batteries. In this work, thin films of LFP, exhibiting a thickness between 200 and 500 nm, were prepared by rf-ion beam sputter deposition. The films were characterized by means of X-ray diffraction (XRD), transmission electron microscopy (TEM), cyclic voltammetry (CV), and galvanostatic intermittent titration technique (GITT). The LFP films were deposited on silicon substrates at different temperatures between 400°C and 700°C. In all cases, TEM

measurements show smooth and homogeneous layers, and XRD results indicate the desired crystalline structure. For detailed electrical characterisation, an additional metallic current collector (Pt, Au) of about 100 nm was deposited, so the electrochemical functionality of the samples could be investigated. First CV results show that the deposition temperature strongly influences the electrochemical capacity, and that a temperature of around 500°C results in LFP thin films of a maximum storage capacity of about 60 mAh/g. Since the thin films reveal a well-defined thickness, they give the possibility to precisely determine the diffusion coefficient of lithium in LFP by means of GITT. So, the diffusion coefficient as a function of the lithium concentration was determined, using the GITT thin film approach.

MM 17.34 Mon 17:00 Poster B

Investigation of freeze casting at the microscopic scale — •Marcel Huber[1], Frank Wendler[2], and Britta Nestler[1,2] — [1]IAM-ZBS, Karlsruhe Institute of Technology — [2]IAM-ZBS, Karlsruhe University of Applied Science

Motivated by freeze casting, an established process to produce ceramic materials with an open pore structure, we study ice crystal growth by using a phase-field model of Allen-Cahn type. The representation of each ice-crystal of different orientation and the liquid is defined by introducing non-conserved order parameters. The solid/liquid interfaces evolve due to an interplay of a driving force and of interface anisotropies with a normal velocity depending on a chemical potential, kinetic coefficient and surface stiffness. We present an anisotropy formulation for interface energies and kinetics suitable for ice-crystallization by a combination of selected spherical harmonics. We introduce an efficient numerical method based on the definition of appropriate boundary conditions to solve the dynamics of the thermal field. We show the dendritic growth shapes and evaluate the tip velocities. We investigate the solidification of ice in a pure water-ice system where water freezes by cooling from one side (cooling plate). By changing the temperature gradient, we evaluate the velocity of the solid/liquid interfaces and compare our results with experimental observations. With regard to the freeze casting process, we analyse the freezing process in a water system filled with inert particles. In simulations, we study the interaction of the particles with the growing ice front and among each other.

MM 17.35 Mon 17:00 Poster B

Silicon nanowires as anode electrodes for lithium ion batteries — •Gibaek Lee[1,2], Stefan L Schweizer[2], and Ralf B Wehrspohn[1,2] — [1]Fraunhofer Institute for Mechanics of Materials Halle — [2]Martin-Luther-University Halle-Wittenberg

It has been known for some time that silicon can incorporate large amounts of Li with a specific capacity of 4200 mAh/g, about a factor of 11 larger than for state of the art graphite anodes. However, silicon and silicon-based negative electrodes exhibit huge volume expansion (ca. 270%) during lithium insertion and extraction, resulting in mechanical disintegration of electrode and rapid capacity fading. One way to overcome the problem of large volume expansion is to design three-dimensional porous electrode structures with sufficient porosity to accommodate the volume expansion. In this study, we prepared oriented silicon nanowire arrays (SiNWs) on n-type silicon substrate by metal assisted chemical etching in aqueous HF solution containing AgNO3. In addition, to reduce the usage of thick silicon substrates and extend applications of silicon micro/nanostructures on various substrates, we have developed ways to detach these SiNWs from bulk silicon substrate because particularly, the contribution of silicon wafer substrate could not be excluded from the capacity of the anode substrate.

MM 17.36 Mon 17:00 Poster B

Surface changes of defect-rich Palladium films under hydrogen atmosphere — •Marc Waninger and Astrid Pundt — Instiute of Material physics, University of Goettingen Friedrich-Hund-Platz 1, D-37077 Goettingen, Germany.

Because of the large out-of-plane expansion of thin films during hydride formation, phase transformation can be studied by surface analyses.[1] In this paper, we artificially generate surface-defects and study their influence on hydride formation by means of atom force microscopy (AFM).

200 nm Palladium films, prepared by ion-argon-beam sputtering at room temperature, are indented by an AFM Cantilever using different loads. Thereby, indentation craters of different size and shape are generated. Subsequent surface changes during hydrogen loading are studied by performing AFM measurements in a gas loading setup.

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

[1] K. Nörthemann and A. Pundt, Phys. Rev. B 78, 014105 (2008), Phys. Rev. B 83, 155420 (2011)

MM 17.37 Mon 17:00 Poster B

Atomistic Multi-Time-Scale Modelling of Cu-alloyed α-Fe — •David Molnar[1,2], Peter Binkele[1], Stephen Hocker[1], and Siegfried Schmauder[1,2] — [1]Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart — [2]Stuttgart Research Centre for Simulation Technology (SRC SimTech), SimTech Cluster of Excellence, University of Stuttgart

Cu-alloyed α-iron changes its material behaviour during its ageing process, especially when operated at higher temperatures of above 300°C, due to Cu-precipitates forming on a relatively large time scale within the Fe-matrix. In order to model this complex behaviour, the growth process of precipitates is accounted for by a Kinetic Monte-Carlo (KMC) approach. Several different precipitation states are transferred from KMC as starting configurations to Molecular Dynamics (MD) simulations allowing for nano tensile tests at different stages of the precipitation process and hence at relevant precipitation times. This can be understood as a multi-time-scale approach in a sequential way. Focusing onto single crystals to reveal the sole effect of the precipitates on the mechanical material behaviour, different structural orientations of the α-iron matrix are investigated in order to obtain an anisotropic temporal behaviour of, e.g., Young's modulus. Thus, the combination of the methods bridges the short time scale of MD with the longer time scale accessible with KMC simulations. In this way, a computational modelling of tensile tests throughout an ageing process of Cu-alloyed α-Fe is achieved as a step towards multiscale-simulation-based design of materials with desired properties.

MM 17.38 Mon 17:00 Poster B

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

A new cluster deposition system for the synthesis of materials composed of mass-selected clusters embedded in matrices of other materials as well as cluster-decorated surfaces was constructed. This approach can open pathways to a new class of materials with tailored electronic, magnetic or catalytic properties.

The clusters are prepared in a source that combines magnetron sputtering and gas-phase aggregation. This allows the production of clusters of various materials with sizes ranging from a few atoms up to several nm. The ionized clusters are first shaped into an ion beam, then mass selected in a 1.4 T sector magnet and finally deposited on a substrate with deposition energies ranging from 0.1 to 100 eV/atom. This covers the whole range from soft-landing up to energetic impact conditions at which the clusters are immobilized and embedded in the substrate. The matrix material can be optionally co-deposited using a high temperature effusion cell or an electron beam evaporator. Altogether the new system is a versatile instrument to synthesize nearly every type of cluster-based materials.

MM 17.39 Mon 17:00 Poster B

Coating Nanoporous Gold by pulsed electrodeposition — •Tobias Kitzler[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Germany

Over the last two decades nanoporous metals produced by selective dealloying have attracted lots of attention. Due to their enormous surface to weight ratio they exhibit outstanding electrochemical properties with respect to their mass/volume. Recently nanoporous materials became more and more interesting for battery applications not only due to their electrochemical properties, but also due to their elastic properties, i.e. the extended elastic range which might be helpful with respect to the cycle stability of the electrodes. To make the nanoporous metal applicable for different usages, e.g. Li storage, it would be interesting to produce nanoporous metals with a coated surface. Successful attempts of such a synthesis were usually limited to very thin coatings or even monolayers.

This work is about the synthesis of nanoporous Au coated with Sn by electrodeposition. The deposition of more than a monolayer is a challenging task. This probably is caused by the low mass transfer rate into the bulk of a nanoporous sample by the electrolyte. In order to circumvent those difficulties, a pulsed electrodeposition method under

a continous electrolyte flow is used. By this method, the electrolyte inside the nanoporous metal is exchanged after each pulse. The samples then were characterised by SEM and EDX and the influence of the system parameters on the electrodeposition process was investigated.

MM 17.40 Mon 17:00 Poster B

On the Interpretation of ELNES - Spectra in the $Al_{1-x}Ti_xN$-System — •Simon Lamowski, Torsten Weissbach, and Jens Kortus — TU Bergakademie Freiberg Institut für Theoretische Physik, Leipziger Str. 23, 09596 Freiberg, Germany

In the particular system studied here layered structures were characterized by Electron energy-Loss Near Edge Structures (ELNES) measurements scanned along a perpendicular direction with respect to the interface.

By means of ab initio Density Functional Theory (DFT) calculations using a Projected Augmented plane Wave (PAW) basis set as implemented in the Abinit code we investigate structural and electronic factors which influence the ELNES. Further , we go beyond standard DFT by solving the Bethe * Salpeter - Equation to obtain the ELNES - spectra using the YAMBO package.

MM 17.41 Mon 17:00 Poster B

Simulation of diffusion processes in Ni and Al, due to the vacancy mechanism in metals on the basis of effective medium theory — •Sergiy Zamulko, Dmitriy Kropachev, and Ganna Kholmska — National Technical University of Ukraine 'Kyiv Polytechnic Institute', Kyiv, Ukraine

In our work we calculated vacancy diffusion processes in nickel and aluminium that based on the effective medium theory. The computer modeling based on the effective medium theory and Atomic Simulation Environment software. The methodic of vacancy diffusion coefficient calculations in metals that based on the effective medium theory has been developed. The computer modeling of vacancy self-diffusion processes in nickel and aluminium has been carried out using the effective medium theory. It has been stated that self-diffusion coefficient of nickel is $0{,}58*10^{-17}$ m^2/s, selfdiffusion coefficient of aluminium is $0{,}3*10^{-12}$ m^2/s. Obtained results can be used for the further calculations of diffusion processes in metal materials on the base of the effective medium theory. And also using of effective medium theory allow accelerating the time for calculations comparing to classical DFT methods.

MM 17.42 Mon 17:00 Poster B

Interaction of Ultrashort XUV pulses with Bulk Magnesium and Copper — •Naira Grigoryan, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University Kassel, Heinrich-Plett-Str. 40, Kassel, Germany

The excitation of a material with very intense femtosecond XUV pulses first leads to an exotic state characterized by a very high density of core holes (about 1 core hole per atom) and relatively warm electrons [Nagler et al.]. The next step is the formation of warm dense matter. In this work we perform all-electron ab initio calculations in order to determine the main pathways from solid to warm dense magnesium and copper. Surprisingly, frozen phonon calculations for the transverse and longitudinal modes at the M point lying at the boundary of the Brillouin zone of magnesium reveal hardening as a function of the electronic temperature in the laser-excited state for LO, LA, TO(perp), TA(perp) and softening for TO(parallel), TA(parallel), and hardening for all modes, as a function of temperature, in the presence of a core-hole. For the copper TA mode at the X point we also find hardening as a function of the electronic temperature in the laser-excited state and in the presence of a core-hole, which is opposite to the behavior of most materials, which soften in at least some directions when electrons are excited.

MM 17.43 Mon 17:00 Poster B

Study of viscoelastic properties of nanoporous gold using dynamic mechanical analysis — •Nadiia Mameka[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, 21502 Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, 21073 Hamburg, Germany

Nanoporous (np) metals fabricated by alloy corrosion have attracted a considerable attention due to their high specific surface area and open nanoligament structure, which can be modified chemically or electrochemically. Unlike bulk nanocrystalline materials, here one can expect not only size-dependence effects of mechanical properties but also significant influence of capillary forces on the elastic and plastic behavior. Recently, it was shown that the mechanical strength of np-Au imbibed with electrolyte can be changed by a factor of 2 by controlling the electrode potential [1]. The aim of this study is the investigation of the change of elasticity of np metals in response to potential changes. We present in-situ experiments in a dynamic mechanical analysis device equipped with an electrochemical cell. The measurements were carried out while electric potentials are applied to a np-Au sample immersed in an electrolyte. Measured storage and loss moduli as well as the damping coefficient upon changing the surface state are discussed.

1. H.J. Jin, J. Weissmüller, Science, 332, 1179 (2011).

MM 17.44 Mon 17:00 Poster B

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

Hydrogen absorption behavior was investigated by in-situ XRD for nano-crystalline Mg thin films at room temperature. Nanocrystalline Mg films with 20nm-thick Pd capping layer were prepared in an UHV chamber, by means of ion beam sputter deposition. XRD measurements using a Phillips X-Pert diffractometer with Co-K alpha radiation were performed before and after hydrogenation to check the phase transition and the change of the sample texture. Thickness changes of films before and after hydrogenation were measured by a Dektak 150 profiler in order to monitor the volume change due to the hydride formation. In-situ XRD measurements have been done at synchrotron facilities. Changes of the resistivity during hydrogenation were also monitored by four-point measurement, during hydrogen gas-loading at several pressures. Reaction kinetics of nano-crystalline Mg thin films with hydrogen at room temperature is estimated from in-situ synchrotron XRD measurements and compared with the results of in-situ electrical resistivity measurements and electrochemical hydrogen permeation measurements. Financial support by the DFG via PU131/9, HASYLAB and ESRF is gratefully acknowledged.

MM 17.45 Mon 17:00 Poster B

Combining ab initio with data mining techniques: Solution enthalpy of hydrogen in transition metals — •Ugur Aydin, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Combining ab initio calculations with data mining techniques we identify a master curve for the solution enthalpy of H in 3d transition metals and related materials. Assuming nonmagnetic fcc crystal structures we find two different classes of materials, with either the octahedral or the tetrahedral interstitial site being preferred by hydrogen. An interaction radius for H in octahedral (tetrahedral) site of ≈ 0.7 Å (≈ 0.4 Å) turns out to be a characteristic value, for which the chemical interaction energy has an optimum for all studied elements. These trends are explained in terms of fundamental band structure parameters.

MM 17.46 Mon 17:00 Poster B

Study of field evaporation from metal tips by using a custom tunable laser-assisted field ion microscope (FIM) — •Armin Feist[1,2], Johannes Endres[1], Carsten Nowak[2], and Claus Ropers[1,2] — [1]University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for Materials Physics, 37077 Göttingen, Germany

In the recent past, field ion microscopy (FIM) and atom probe tomography (APT) have shown their potential as versatile tools for studying materials interacting with ultrashort laser pulses at an atomic scale. In order to examine the physical processes involved in laser-assisted field evaporation from nanoscale tips, a conventional FIM was equipped with a tunable femtosecond laser system. We study the evaporation by differential image analysis in FIM mode, as opposed to direct detection of evaporated sample atoms as in APT. The advantage of this approach lies in its capability to atomically resolve the surface structure during the continuous evaporation process. Wavelength, static field and fluence dependent measurements on W and Mo yield insight into the microscopic evaporation mechanism and support thermal activation, while being inconsistent with the optical rectification model.

MM 17.47 Mon 17:00 Poster B

Band structure und electronic transport properties of cobalt decorated carbon nanotubes — Jan Sommer[1], •Andreas

Zienert[2], and Jörg Schuster[3] — [1]Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, 09126 Chemnitz, Germany — [3]Fraunhofer Research Institution for Electronic Nano Systems, 09126 Chemnitz, Germany

Carbon nanotubes (CNTs) are promising candidates for replacing copper wires in novel interconnect structures. For such an application, it is necessary to use metallic CNTs in order to compete against conventional copper technology. However, only one third of the CNTs grown by chemical vapor deposition are metallic. A method for turning semiconducting CNTs into metallic ones would be highly desirable [1].

As a simple approach, we modeled the effect of a few cobalt atoms, placed on the surface of a semiconducting CNT, on band structure and transport properties by using density functional theory. Even a very small amount of cobalt could significantly alter the band structure by inducing spin polarized states near the Fermi energy. Transport calculations confirm, that the conductivity of the semiconducting single-wall CNT is significantly increased. Furthermore, we present results about the geometry of the cobalt decorated CNT and the influences on band structure and transport.

[1] Kim et al. ACS Nano 3, 2818 (2009)

MM 17.48 Mon 17:00 Poster B

nanoscale solid-solid dissolution of crystalline/amorphours nanoparticles by electron beam irradiation — •Tao Feng[1,2], Di Wang[1], Ralf Witte[1], Robort Kruk[1], Horst Hahn[1], and Herbert Gleiter[1] — [1]Karlsruhe Institute of Technology, Institute for Nanotechnology, Karlsruhe, Germany — [2]Engineering Research Center for Nanophotonics & Advanced Inst6rument, Ministry of Education, Department of Physics, East China Normal University, Shanghai, China

The diffusion behavior between different chemical composition nanoparticles is very critical for understanding the performance stability and lifetime of nanoparticles. Here, we report a systematic study carried out "in-situ" in the transmission electron microscopy (TEM) on an electron-irradiation-induced transformation of crystalline Pd/amorphous $Fe_{25}Sc_{75}$ core/shell nanoparticles, which are prepared by co-evaporation Pd metal and $Fe_{45}Sc_{55}$ alloy in an inert gas condensation (IGC) system. Under the low electron beam irradiation (below 1×10^6 electrons $nm^{-2}s^{-1}$), the crystal lattice of Pd disappeared gradually, accompanying with the growth of Pd domain. High-sensitivity energy-dispersive X-ray (EDX) spectroscopy give the direct evidences of the atomic diffusion between Pd and Sc, which cause to form an new amorphous compound of PdFeSc in the core/shell nanoparticles. Such physical manipulations of nanoparticles can be exploited as a tool to access novel nanoglass.

MM 17.49 Mon 17:00 Poster B

Compositional changes during phase separation of $\gamma\prime$ precipitates in a Ni-Al-Ti model alloy — •Florian Vogel, Nelia Wanderka, and John Banhart — Helmholtz Zentrum Berlin GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The phase-separation phenomenon of $\gamma\prime$ precipitates in a single crystal Ni-8.5Al-5.4Ti (at.%) model alloy was investigated by means of transmission electron microscopy (TEM) and three-dimensional atom probe (3D-AP). After homogenization, ageing at 1213 K led to formation of the initial $\gamma/\gamma\prime$ microstructure composed of cuboidal $\gamma\prime$ precipitates embedded in a γ matrix. Subsequent ageing at 1023 K resulted in the formation of new particles within the $\gamma\prime$ precipitates. Ex-situ TEM was used to follow the influence of these particles on the evolution of microstructure and the kinetics of $\gamma\prime$ coarsening. 3D-AP revealed the chemical composition of the γ matrix, the $\gamma\prime$ precipitates and the particles within $\gamma\prime$. It was found that the particles are rich in Ni and poor in Ti as compared to the $\gamma\prime$ precipitates. The results are discussed with respect to the solubility of Ni within the $\gamma\prime$ phase based on heat treatment conditions.

MM 17.50 Mon 17:00 Poster B

Heat capacity of aluminum nitride phases from *ab initio* calculations — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The ability to calculate thermodynamical material properties on *ab initio* level is an important preliminary for the accurate prediction of phase diagrams.

We present results on the heat capacity of the wurtzite and rocksalt phases of aluminum nitride. The isochoric heat capacity C_V is obtained from harmonic phonon calculations using density functional perturbation theory. In the quasi-harmonic approximation, the isobaric heat capacity C_p is then obtained from C_V via the thermal expansion coefficient. Comparisons of volume expansion coefficients and C_p-values with experiment for the wurtzite phase show the accuracy of the method.

We would like to thank the DFG for financial support within the DFG Priority Program 1236: *Strukturen und Eigenschaften von Kristallen bei extrem hohen Drücken und Temperaturen*

MM 17.51 Mon 17:00 Poster B

Influence of Quenching & Partitioning on martensite and austenite phase composition in steel — •Karin Rüster[1], Andre Steffen[1], Michael Paulus[1], Christian Sternemann[1], Metin Tolan[1], Niko Grosse-Heilmann[2], Christian Kronholz[2], and Andreas Peters[2] — [1]Fakultät Physik / Delta, TU Dortmund, Germany — [2]Benteler Tube Management GmbH, Paderborn, Germany

Steel is a common material in our daily life. Macroscopic characteristics (e.g. hardness, tensile properties...) of steel are affected by the crystalline structure, i.e. austenite and martensite phase, which is changed during heat treatment. During the process of Quenching and Partitioning carbon diffuses from martensite to austenite, enriches the austenite and thereby stabilises the phase of austenite. This way a microstructure with retained austenite is produced. To analyse the influence of heating and cooling XRD-experiments have been carried out, ex-situ for pre-treated samples and in-situ. The experiment was performed at beamline BL9 at Delta.

MM 17.52 Mon 17:00 Poster B

Microstructure of InAs nano-crystals embedded in Si — •Mingjian Wu[1], Achim Trampert[1], Tariq Al-Zoubi[2], Muhammad Usman[2], Mohamed Benyoucef[2], and Johann Peter Reithmaier[2] — [1]Paul-Drude-Institut für Festköperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany — [2]Institute of Nanostructure Technologies and Analytics, CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany

In this work, the structural properties of InAs nano-crystals embedded in a Si matrix are investigated by transmission electron microscopy (TEM). The InAs is grown on Si (001) by molecular beam epitaxy at 400 °C and subsequently overgrown by Si at 700 °C. Depending on the nominally deposited amount of InAs, the embedded clusters show spherical and truncated octahedral-like shapes with {111} and {001} facets, which are significantly different to the initially flat InAs islands. The bulk lattice mismatch of 10.4 % is relieved by dislocation loops along the interface consisting of perfect 60°-type dislocations and partial dislocation with stacking faults inside the InAs clusters. By two-dimensional strain mapping derived from high-resolution TEM structure images, no strain gradients in the Si matrix around InAs clusters are detectable. On the other hand, anisotropic lattice distortions inside the InAs clusters are identified, which are characterized by compressive and tensile strain distributions in the two mapped directions, i.e. parallel and perpendicular to the growth direction. This residual strain is discussed based on the thermal mismatch between InAs and Si.

MM 17.53 Mon 17:00 Poster B

Is the epsilon-phase in deformed autenitic steel just an accumulation of stacking faults? — •Torsten Weissbach, Sebastian Schwalbe, Jürgen Kutzner, and Jens Kortus — Institut f. Theoretische Physik, TU BergAK Freiberg, 09596 Freiberg

Highly alloyed TRIP steels consisting of metastable austenite show a transformation induced by deformation to the hexagonal lattice known from the hcp phase of iron. It has been shown by other authors that the X-ray data proving this can also be interpreted as stacking faults, because they usually occur on hexagonal planes in cubic Fe. Furthermore, the stacking fault energy in TRIP steel is low compared to other steel types.

We show density functional theory calculations on Fe to address the question under which conditions the hcp phase can be stable. Because the alloyed steel exhibits considerably strained lattice parameters, we are particularly interested in the behaviour of Fe under such conditions. The Fe phases are a complicated system for DFT; calculations are known to be very sensible to the type of exchange-correlation functional.

MM 17.54 Mon 17:00 Poster B

Gas diffusion electrode development using femtosecond-laser induced microstructured metal surfaces with hydrophobic features — Andreas Gabler[1], Anna-Lena Baumann[1], Thomas Gimpel[2], Stefan Kontermann[1], Robert Hahn[3], and •Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, 38640 Goslar — [2]Clausthal University of Technology, EFZN, EnergieCampus, 38640 Goslar — [3]Fraunhofer Institute for Reliability and Microintegration, IZM, 13355 Berlin

At present, hydrophobic characteristics of gas diffusion electrodes are mostly generated by using polytetrafluoroethylene-materials (PTFE).

An innovative, methodic approach of directly generating new hydrophobic metal surfaces is developed by using femtosecond-laser induced microstructures through ablation, similar to the so called Black Silicon Material.

Its characteristic appearance is a spike-structure at micrometer level, in which superhydrophobic characteristics have already been successfully achieved. Preliminary analyses examined the good usability of the fs-laserprocess in cases of surface structuring on different metals.

The direct generation of microstructured metal surfaces with hydrophobic characteristics for gas diffusion electrodes has the advantage of being a one-material-system with the combined features of hydrophobicity, electrical conductivity und large catalyst surface at a three phase boundary .

In this case, different process settings were made and the resulting surface structures and hydrophobic characteristics compared.

MM 17.55 Mon 17:00 Poster B

In-situ observation of structural changes accompanying lithium intercalation in silicon TEM lamellas — •Timo Wuttke, Burkhard Roos, Carsten Nowak, and Cynthia Volkert — Georg-August-Universität Göttingen, Institut für Materialphysik

In-situ studies of electrochemically driven lithiation and delithiation of materials for lithium-ion-batteries promise an improved understanding of the underlying intercalation mechanisms. We report the construction of a miniature lithium-ion-battery inside a transmission electron microscope using a STM-TEM holder. The cathode consists of a $LiMn_2O_4$-particle, while a silicon TEM lamella is used as anode. A liquid electrolyte ensures a high ionic conductivity between both components. It is based on an organic conducting salt dissolved in an organic ionic liquid and has a very small vapor pressure, enabling its use in the high vacuum of a TEM.

Crystalline silicon experiences several phase transitions with increasing amount of lithium and is amorphous once fully lithiated. Structural changes of both cathode and anode during lithiation are studied. Current-voltage characteristics, volume expansion and amorphization during lithiation are discussed.

MM 17.56 Mon 17:00 Poster B

Lithium ion dynamics in channel-structured $Li_2Ti_6O_{13}$ — •Kai Volgmann and Paul Heitjans — Leibniz Universität Hannover, Inst. f. Phys. Chemie u. Elektrochemie, Callinstraße 3 - 3a, D-30167 Hannover

Solid-state nuclear magnetic resonance (NMR) spectroscopy subsumes a couple of powerful techniques to investigate the diffusion of Li ions on the microscopic scale. These methods can be used, e. g., to investigate effects on the motion of Li^+ ions by dimensionality reduction. In this work, $Li_2Ti_6O_{13}$ (space group C m/2) has been chosen as model system due to its channel-like crystal structure. Lithium is supposed to be solely located inside the channels. Samples with varying Li content have been studied. Synthesis is done via a solid-state reaction and subsequent ion exchange of sodium ions. The samples were characterized by powder x-ray diffraction and inductively coupled plasma optical emission spectroscopy. ^{7}Li NMR relaxometry measurements have been performed at different Lamor frequencies ω_0. Due to the channel-like structure, a confined Li diffusion process is expected leading to a frequency-dependent spin-lattice relaxation rate in the regime $\omega_0 \cdot \tau \ll 1$ where τ is the motional correlation time. A blocking effect in the structure due to the sodium cations is observed for samples with substoichiometric Li concentration.

MM 17.57 Mon 17:00 Poster B

Molecular Dynamics Simulation of Aluminum Oxidation via Reactive Force Field — •Manana Koberidze and Risto Nieminen — Aalto University, School of Science, Espoo, Finland

Tunneling current in aluminium-oxide thin film based nano-electronic devices is strongly dependent on the geometry of a metal-oxide interface [1], affecting the quality of the barrier, consequently, performance of a device. Therefore, it is crucial to know the structure of the interface and kinetics of its formation. Most of the works addressing aluminum oxidation consider only initial stages at low coverage. Rather little information is available about the interfaces in question.

Our goal is to achieve detailed understanding of oxide growth via molecular dynamics simulations, further, to develop quantitative description of transport relevant barriers. We use Reactive Force Field (ReaxFF) [2] which has been successfully exploited for Al/Al_2O_3 interface and is claimed to be fully transferable for the description of oxidation process [3]. Simulated results for Al(111) oxidation above one monolayer coverage will be presented. Calculations are performed in the near-room-temperature range, thereby assessing the applicability of ReaxFF to the current problem.

References:
[1] V.F. Maisi, et al., PRL 106 (2011) 217003.
[2] A.C.T. van Duin, et al., J. Phys. Chem. A 105 (2001) 9396.
[3] Q. Zhang, et al., Phys. Rev. B 69 (2004) 045423.

MM 17.58 Mon 17:00 Poster B

An approach for quantitative assessment of shear induced mixing in mechanical alloying — •Mohsen Pouryazdan[1], Di Wang[1], Torsten Scherer[1], Robert Averback[2], and Horst Hahn[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021, Karlsruhe, Germany — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, 1304 W. Green St., Urbana, IL 61801, USA

A critical feature in the processing of nanocomposites is the forced mixing of alloying components. By forced mixing we refer to the atomic mixing of atoms attributed to shear deformation. Presently, this process is only poorly understood. This lack of understanding is partly because nearly all of our information to date has been derived from experiments employing ball milling (BM), for which the mixing conditions: strain rate, total strain, temperature, and stress state are poorly characterized. In contrast to experiments using BM, our experimental approach using high pressure torsion (HPT) allows quantitative assessment of mixing conditions. In the current study, Ag60Cu40 two-phase immiscible alloy was processed by HPT for various levels of strain. The state of intermixing was investigated by XRD, DSC and TEM.

It is observed that the rate of chemical disordering increases with the accumulation of applied strain. A complete chemical homogenization of the original lamellar structure of Ag60Cu40, with periodicity of ~165 nm, is achieved after a shear strain of ~725 at a shear strain rate of ~1.5 1/s. The chemical mixing is accompanied by extensive grain refinement leading to nanocrystalline grains with average size of ~42 nm.

MM 17.59 Mon 17:00 Poster B

Origin of high Neel temperatures in Tc perovskites — Jernej Mravlje[1,2,3], Markus Aichhorn[4], and •Antoine Georges[1,2] — [1]College de France, Paris, France — [2]Ecole Polytechnique, Palaiseau, France — [3]Josef Stefan Institue, Ljubljana, Slovenija — [4]TU Graz, Austria

Very recently, antiferromagnetism persisting to high temperatures exceeding 1000K was discovered in Tc perovskites. Usually, robust magnetism is associated to 3d transition metal oxides, moreover in 4d oxides magnetism is rarely found. Here we describe results of LDA+DMFT calculation of electronic structure of two cubic perovskites, SrMnO3 and SrTcO3. The Neel temperature of SrTcO3 is found 4 times larger, in agreement with experiment. Smaller Tc moment is reproduced aswell. We show that the distinction between the two materials is that Tc is far more on the itinerant side, and found in the immediate proximity to the metal-insulator transition in the paramagnetic state. Accordingly, the dependence of Neel temperature on pressure is very weak in strong violation of the Bloch's law.

MM 17.60 Mon 17:00 Poster B

Hybrid material design with DFT: Silane coupling agent on TiO_2(011) — •Wolfgang Heckel, Beatrix Elsner, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

In order to control the mechanical properties of hybrid materials, the detailed knowledge of the interfaces, the atomic structure and stability is crucial. Density functional theory (DFT) allows for the investigation of the local electronic structure and the determination of desired

observables like binding energy.

Using the TiO_2 bulk rutile structure as a starting point, we develop a model system for the interface between the adsorbing silane coupling agents and the $TiO_2(011)$ surface representing a ceramic-polymer junction. Here, a good choice for the exchange-correlation functional plays an essential role. We find that the release of bonding energy depends heavily on the adsorption sites and the energetically most favourable molecular arrangements show only weak bonding to the surface. The tendency of the adsorbing molecules to form clusters before adsorption will be discussed.

MM 17.61 Mon 17:00 Poster B

Simulation of structural phase transitions and shape memory behavior in NiTi nanosystems — •Daniel Mutter and Peter Nielaba — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

We present results of atomistic molecular dynamics simulations of structural phase transitions and shape memory behavior of NiTi nanosystems. The application of heating-cooling cycles to bulk systems (2000 atoms under periodic boundary conditions) confirmed the experimentally known strong dependence of B19'-to-B2 transition temperatures (TTs) on alloy composition, which could be related to an increasing lattice instability, arising when the perfect ordered composition with 50% Ni and 50% Ti is changed slightly [1]. By applying free boundary conditions, spherical NiTi nanoparticles are simulated, showing a size dependence of the TTs. Further calculations suggest this to be due to an increasing surface-to-volume fraction and therefore a major influence of the surface free energy when the system size is reduced [2]. In addition, the nanoparticles show twinning of differently orientated variants of a B19'-like structure at low temperatures. We apply loading-heating-cooling cycles to these systems, which shows a shape memory behavior at the nanoscale differing from the known bulk mechanism.

[1] D. Mutter and P. Nielaba, Phys. Rev. B 82, 224201 (2010).
[2] D. Mutter and P. Nielaba, Eur. Phys. J. B 84, 109 (2011).

MM 17.62 Mon 17:00 Poster B

Modeling the crystal growth phenomena on atomistic scale in single crystals and binary alloys — •Muhammad Ajmal Choudhary[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Institut für physics, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

The phase field crystal (PFC) technique is a novel approach for modeling crystal growth phenomena with atomistic resolution. Here we demonstrate the derivation of an anisotropic phase-field crystal (APFC) model, recently elaborated and investigated by M A Choudhary et al. [J. Phys.: Condens. Matter 23, 265005 (2011)] from microscopic density functional theory for anisotropic particles. We explored its crystal morphologies to demonstrate the influence of anisotropy and undercooling on nucleation and microstructure formation process. These stable phases are also investigated with respect to their characteristic morphological features. To describe the equilibrium properties of eutectic binary alloys in two dimensions, we develop a simple binary PFC model based on Elder et al. [Phy. Rev. B 75, 064107 (2007)]. We implement it as a real space dynamic code in two dimension. We analyze properties of metastable nuclei in the liquid-solid co-existence region and just below the eutectic point using the technique of finite system size phase transitions [Phy. Rev. E 79, 061104 (2009)]. Of particular interest is the growth of a secondary solid phase on a primary nucleus occurring during eutectic solidification.

MM 17.63 Mon 17:00 Poster B

Simple Synthesis of Metal and Metal Oxide Nanowires for Device Application — •Pervin Sahin, Necdet Onur Urs, Dawit Gedamu, Torge Behrendt, and Rainer Adelung — Functional Nanomaterials, Institute for Material Science, Faculty of Engineering, University of Kiel, Germany

1-dimensional metal and semiconductor nanostructures exhibit interesting physical properties but their integration into modern electronic devices is often a very challenging task. Finding the appropriate supports for nanostructures and nanoscale contacts are highly desired aspects in this regard. In present work we demonstrate the fabrication of 1D nano- and mesostructures between microstructured contacts formed directly on a silicon chip either by a thin film fracture (TFF)[1] approach or a delamination approach. Both approaches offer the possibilities to integrate the obtained nano- meso structures in wafer level fabrication. Recently, a novel approach named hot plate delamination approach allowed to fabricate connected single crystalline iron oxide nanowires from delaminated and microstructured iron films in a self organized way on a hot plate. Electrical properties of these nano-micro structures integrated on Si-chips and their preliminary applications towards sensors and field effect transistors are presented as well.

[1]Dawit Gedamu, Ingo Paulowicz, Seid Jebril, Yogendra Mishra, and R. Adelung, Journal of Nano Technology, October 2011(in press)

MM 17.64 Mon 17:00 Poster B

Exploring GPUs for Mesoscale Simulations — •Alexander Monas, Claas Hüter, and Robert Spatschek — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The modeling of microstructure evolution like solidification or solid state transformations as well as many other pattern formation processes in general requires the solution of coupled partial differential equations. This is in particular the case for phase field modeling, where the motion of phase fronts is represented by the temporal evolution of an order parameter field. These simulations are very time consuming, and therefore frequently massive parallelization is used to accelerate the computations. Here we report on implementations on (consumer) graphics cards, which have a theoretical peak performance of more than 1 TFlop. We demonstrate the efficiency of this approach for diffusion problems and phase transformation processes, where we use real space implementations in two and three dimensions. For amplitude equation models, which are derived from classical density functional theory, we use pseudospectral methods. The efficiency of the GPU implementations is shown for solid-liquid interface interaction and for dislocation pairing transitions at hot grain boundaries.

MM 17.65 Mon 17:00 Poster B

Hydrogenation of Magnesium Titanium Multi- Layers — •Jara Kürschner, Helmut Uchida, and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Freidrich-Hund-Platz 1, 37077 Göttingen

Magnesium is a promising metal for hydrogen storage as it can store up to 7.6 weight% H. But, its hydrogen sorption kinetics are very slow. Magnesium can be combined with metals such as titanium, which have fast hydrogen sorption kinetics and do not alloy in equilibrium.

In this work, the hydrogen absorption properties of different magnesium titanium multi-layer stacks are investigated by electrochemical loading at room temperature. The palladium-capped samples are prepared by ion beam deposition on cleaned substrates and structurally analysed by X-ray diffraction.

Their properties such as hydrogen pressure and transmittance are analysed in dependance of the connection to the substrate and the Pd cap, the layer stacking, and the layer thickness.

This research is kindly supported by DFG PU131/9.

MM 17.66 Mon 17:00 Poster B

Interfaces in Fe/MgO/Fe sandwich structures — •Torben Boll[1], Talaat Al-Kassab[1], Catharina Wille[1], and Ryota Gemma[2] — [1]King Abdullah University of Science & Technology, Division of Physical Sciences, Thuwal, Kingdom of Saudi Arabia — [2]Institut für Materialphysik, Göttingen, Germany

Electronic devices, based on the Tunnel Magneto-Resistance (TMR) effect, which are consisting of multi layered structures, are of emerging interest. The magnetic properties of such multilayer structures are governed by the properties of the metal/oxide interfaces. This paper focuses on Atom Probe Tomography (APT) investigations of the interfaces in such multilayer structures.

Fe/MgO/Fe/Au layer structures were deposited on Si-microtips by Ar-sputtering. The Au-layer is meant to prevent oxidation when the sample is exposed to the air. Results of different thermal treatments will be presented in this study to elaborate the mixing effects at the metal/oxide interface. The APT measurements were performed with the LEAP 4000 HR at the King Abdullah University of Science & Technology.

MM 17.67 Mon 17:00 Poster B

Analysis of the nitrogen content of carbide particles in a gamma'-strengthened Ni-based superalloy — •Martin Peterlechner, Harald Rösner, and Eckhard Nembach — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm Klemm Straße 10, 48149 Münster, Germany

Ni-based superalloys are commercial construction materials used at el-

evated operating temperatures. Carbide particles contribute to their mechanical properties. In the past these carbides were referred to as carbo nitrides but it is a question of long standing whether they do contain nitrogen and if so in what concentration. We have examined the nitrogen content of carbide particles of (Ti,Mo)-C carbides in a commercial superalloy (NIMONIC PE16) by electron energy loss spectroscopy (EELS) and energy dispersive X-ray analysis (EDX). The results suggest that the content of nitrogen in these carbides is negligible.

MM 17.68 Mon 17:00 Poster B

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

The oscillation behaviour of Silicon nanomechanical resonators in the form of doubly clamped beams is investigated by Molecular Dynamics simulations using the Stillinger-Weber interaction potential. After setting up the initial structure using a diamond lattice and a (2×1) symmetric dimer surface reconstruction, the end points of the beams are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the beams. Besides varying the size of the beams, the effects of temperature and external stretching fields are explored. The results show a decrease of the oscillation frequencies with rising temperature and a strong increase of the damping coefficient, a strong increase of the frequencies with external stress (stretching) and a decrease of frequencies with length. Other materials (e.g. NiTi memory alloys) are explored as well.

MM 17.69 Mon 17:00 Poster B

Hydrogenation behavior of thin epitaxial Nb films: Film preparation and hydrogen gas loading — •Vladimir Burlaka[1], Stefan Wagner[1], Anthony Bell[2], and Astrid Pundt[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]HASYLAB Hamburg, Germany

For thin films below a critical film thickness it was reported [1,2] that stress release via the formation of dislocations during hydrogen loading is energetically suppressed. To study this, Nb-H thin films are used as a model system. As a first step, the proper substrate temperatures for atomically smooth and epitaxial Nb film growth of thin films (20nm) on sapphire substrates during UHV sputter deposition were determined. In order to monitor hydride precipitation in the Nb films during hydrogen gas loading, in-situ STM measurements for 20 nm film thickness were performed, characterizing the films surface morphology in the as prepared and in the hydrogenated state.

Hydrogen induced lattice parameter changes of the Nb films were investigated by in-situ X-ray diffraction measurements during hydrogen gas loading at the synchrotron radiation facility in HASYLAB, Hamburg. It was shown that for a film with 20 nm, peak shifts change. We interpret this with a reduced dislocation formation.

[1] K. Nörthemann, A. Pundt, PHYS. REV. B 78, 014105 (2008)

[2] S. Wagner, H. Uchida, V. Burlaka et al., Scripta Materialia, Vol.64, Issue 10, p. 978-981 (2011)

This research was kindly supported by the DFG via PU131/9-1 and HASYLAB via project II-20060117.

MM 17.70 Mon 17:00 Poster B

Atomic scale simulations of elastic properties of Al_2O_3–C refractories — •Yuriy Natanzon and Heike Emmerich — Lehrstuhl für Material- und Processsimulation, Universität Bayreuth, Nürnberger Str. 38, 95448 Bayreuth, Germany

Aluminium oxide has a lot of significant industrial applications, in particular Al_2O_3 with 4% carbon addition is used as a refractory material. In this respect the influence of nano-additives on the elastic properties of this material is crucial to understand the phenomenon of crack propagation and fracture on atomic level. In addition, atomic scale calculations can be used as a starting point for studying this phenomenon on the macroscale. In particular, calculated elastic constants are further used for the phase field simulations of the crack propagation in ceramic refractories.

Here we present the results of molecular dynamics simulations of the dynamics of crack propagation in carbon doped α–Al_2O_3 refractories. As such simulations are time consuming, we obtain the relaxed crystal structure by means of classical molecular dynamics, and then materials properties are calculated by the combination of density functional theory and molecular dynamics. The dependence of elastic properties on both temperature and carbon content is analyzed. Our results contribute to the understanding the mechanism of bond breaking and dynamics of crack propagation on the atomic level for the purpose of designing a new fire-proof materials with reduced carbon content.

MM 17.71 Mon 17:00 Poster B

Comparison of MOKE- and SQUID-detected magnetization of FePt-layers on MgO-substrates — •Peter Jerabek[1], Thomas Bublat[2], Dagmar Goll[3], Stefan Topolovec[4], Roland Würschum[4], and Heinz Krenn[1] — [1]Karl-Franzens-University Graz, Graz, Austria — [2]Max Planck Institut für Intelligente Systeme, Stuttgart, Germany — [3]Aalen University, Materials Research Institute, Aalen, Germany — [4]Institut für Materialphysik, TU Graz, Graz, Austria

Chemically ordered FePt in the L10 phase is known as hard magnetic material with an extremely high magnetic anisotropy. From SQUID measurements [1] different mechanisms of magnetization reversal have been recognized: nucleation or pinning of domain walls depending on the layer thickness, on the degree of chemical order and on the grain size distribution. Coherent rotation or domain wiping determines the coercivity. SQUID magnetometry allows to monitor (and calibrate) the in-field- and the the out-of-field magnetization, but the Magnetooptic Kerr Effect (MOKE) provides additional information about the dynamics of magnetization reversal. The enhanced surface sensitivity of MOKE is utilized to account for the electric tunability [2] of magnetization by soaking FePt/MgO-films in KCl electrolyte, for which a special electrochemical cell including a reference electrode is designed.

[1] T. Bublat, D. Goll, J. Appl. Phys. 108 (2010) 113910

[2] M. Weisheit et al., Science 315 (2007) 349

MM 17.72 Mon 17:00 Poster B

Ehrenfest molecular dynamics within the projector augmented-wave method — •Ari Ojanperä[1], Ville Havu[1], Lauri Lehtovaara[2], Arkady Krasheninnikov[1,3], and Martti Puska[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]LPMCN, Université Claude Bernard Lyon 1, France — [3]Materials Physics Division, University of Helsinki, Finland

Modeling nonadiabatic processes, such as ion-atom collisions and electron transfer in molecular and biological systems, represents major computational challenges because multiple potential energy surfaces (PESs) are involved in the dynamics. Consequently, traditional ab initio molecular dynamics (AIMD) methods, founded on the assumption that the electronic subsystem is in its ground state, cannot be used. Ehrenfest molecular dynamics (Ehrenfest MD) within time-dependent density functional theory (TDDFT) offers a computationally affordable approach to simulating nonadiabatic processes by coupling the quantum equations of motion for electrons with classical equations of motion for nuclei via an average potential surface.

We have implemented Ehrenfest MD within the projector augmented wave (PAW) method. The electronic structure program used for the implementation is GPAW, which uses real space grids and finite differences. We demonstrate the applicability of our method by studying electronic stopping in graphene. We find that our PAW-based Ehrenfest MD results agree well with previous Troullier-Martins pseudopotential calculations. Moreover, the agreement with experiments is good as long as the effect of core electron excitations is small.

MM 17.73 Mon 17:00 Poster B

Real structure characterization of shockwave-synthesized γ-$Si_3(O,N)_4$ — •Anke Köhler[1], Christian Schimpf[2], Thomas Schlothauer[3], Volker Klemm[2], Marcus Schwarz[1], Gerhard Heide[3], David Rafaja[2], and Edwin Kroke[1] — [1]Institute of Inorganic Chemistry, TU Bergakademie Freiberg, Leipziger Str. 29, 09596 Freiberg — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Str. 5, 09596 Freiberg — [3]Institute of Mineralogy, TU Bergakademie Freiberg, Brennhausgasse 14, 09596 Freiberg

The spinel-type Si_3N_4 is known since 1999 and is counted among the hardest materials. It can be synthesized under high pressure only. Although the thermodynamic phase boundary is ~ 12 GPa, usually large overpressures are required for shock wave synthesis of larger amounts of the material. The application of amorphous precursors and peak shock pressures ≥ 35 GPa enabled us to manufacture spinel-type material in the system Si-O-N without impurities of the low pressure modifications.

The global chemical composition of the synthesized samples was investigated by means of elementary analysis (EA) and SEM/EDX. The

sample with the most perfect microstructure data obtained by X-Ray diffraction shows the lowest oxygen content. Detailed microstructure analyses of the $Si_3(O,N)_4$-nanopowder using high resolution TEM confirmed the expected spinel structure. However, they disclosed some extended crystal structure defects. EELS measurements showed much broader variation of the [O]/[N] ratios than expected.

MM 17.74 Mon 17:00 Poster B

Characterization Strategies for Material Processing with Structured fs-Laser Pulses — •Conrad Schuster, Anna Svanidze, Neeke Rothe, Steffen Fiedler, Robert Irsig, Anna Oniszczuk, Josef Tiggesbäumker, Karl-Heinz Meiwes-Broer, and Stefan Lochbrunner — Institute of Physics, University of Rostock, Germany

Material processing with ultrashort laser pulses attracts considerable attention since it allows for micro machining with highest precision. The characteristics of both laser pulse and processed material determine plasma formation and the appearance of the subsequent breakdown of the material. To optimize the machining process and to understand the laser material interaction, online characterization methods are highly desirable. For this purpose we have developed two setups, one is to observe the time dependent material response on the laser pulse impact and the other is to characterize the obtained structures at the location of processing. In the first setup the output of a Ti:Sa fs laser system is split into two beams. The first beam passes through a pulse shaper and provides structured NIR pulses for the machining process. The second one is frequency doubled and the resulting blue probe pulses are guided via a delay stage through the same focusing objective as the machining pulses. The transmitted blue light is recorded by a CCD camera to study the evolution of the plasma generated by the NIR pulses. In the second setup the objective for machining is simultaneously used as the front end of a confocal microscope. This enables an online characterization of the generated microscopic structures.

MM 17.75 Mon 17:00 Poster B

NanoSculpt: a tool for generating arbitrarily shaped structures for atomistic simulations — •Martin Hummel[1], Siegfried Schmauder[1], and Erik Bitzek[2] — [1]IMWF, Universität Stuttgart — [2]Dept. Werkstoffwissenschaften, WW1, Universität Erlangen-Nürnberg

Atomistic simulation methods are becoming increasingly popular in the study of mechanical properties of materials. In particular in combination with in-situ experiments they allow the identification and detailed study of deformation mechanism. However, replicating experimentally studied specimens on the atomic scale still is an almost artisanal process. Commonly used approaches include the use of cutting planes or analytical mathematical expressions to generate geometrical shapes, or, in case of polycrystals, the use of Voronoi tessellation. Simulations using such simplified structures are very successful in providing generic information, however the specific deformation mechanisms of particular structures may depend sensitively on theire complex shape. Here we present an open-source software tool to generate complex 3D shapes for the use in atomistic simulations directly from experimental or simulation data. The tool is based on the ray-crossing algorithm from computational geometry to determine whether a given point lies inside a polyhedron. It requires triangulated surface meshes, which are commonly generated by serial sectioning or tomography methods, or can be extracted from grain growth or phase field simulations. Presented examples include grains reconstructed from serial sectioning and experiments, precipitates, nano-foams, and surface structures.

MM 17.76 Mon 17:00 Poster B

Accelerating DFT and TDDFT Electronic Structure Calculations Using Graphics Processing Units — •Samuli Hakala[1], Ville Havu[1], Jussi Enkovaara[2], Martti Puska[1], and Risto Nieminen[1] — [1]Department of Applied Physics, School of Science, Aalto University, Espoo, Finland — [2]CSC - IT Center for Science Ltd., Espoo, Finland

A Modern Graphics Processing Unit (GPU) is an efficient many-core stream processor suitable for throughput-orientated General Purpose (GP) parallel computations. Usage of GPGPU in scientific calculations has increased a lot in recent years. We have accelerated an electronic simulations software GPAW using GPUs. GPAW is a Density Functional Theory (DFT) program package based on the Projector Augmented Wave (PAW) method. Time-Dependent Density Functional Theory (TDDFT) is implemented in the linear response and time propagations schemes. Physical quantities are represented in a uniform 3D real space grid.

We have implemented GPU accelerated versions of the most numerically intensive parts in GPAW calculations using NVIDIA CUDA. Multiple GPUs and cluster nodes can be utilized with MPI using domain decomposition or by parallelizing over k-points. High performance is achieved by hand tuning the CUDA kernels and by minimizing data transfers between the GPU and the host computer. We describe our implementation and analyze the performance and the scalability of the code. Our results show that GPUs can provide significant speed-ups in both DFT and TDDFT calculations.

MM 17.77 Mon 17:00 Poster B

Enhanced Ferromagnetism in Nanometallic Glass studied by Mössbauer spectroscopy — •Ralf Witte[1,2], Tao Feng[1], Mohammad Ghafari[1], Robert Kruk[1], Richard Brand[1], Herbert Gleiter[1], and Horst Hahn[1,2] — [1]Karlsruher Institut für Technologie, Institut für Nanotechnologie, D-76344 Eggenstein- Leopoldshafen — [2]Technische Universität Darmstadt, Gemeinschaftslabor Nanomaterialien, Petersenstr. 23, D-64287 Darmstadt

Interface or grain boundary effects in materials have been widely investigated since the discovery of nanocrystalline materials. In the next step these studies have been extended to another interesting class of materials such as nanoglasses or nanostructured amorphous solids. These materials can be produced by synthesis of amorphous nanoparticles in an inert-gas-condensation (IGC) process and subsequent compaction in UHV. The resulting solid material is characterised by its increased density of structural defects (interfaces) and drastically increased free atomic volume in the interfaces between the glassy nanoparticles. We report on a study using Mössbauer spectroscopy and magnetic property measurements of a nanoglass prepared from amorphous $Fe_{90}Sc_{10}$ nanoparticles. The material investigated exhibits dramatic changes in magnetic properties, namely an increased magnetic transition temperature by more than 200 K and enhanced magnetic hyperfine fields compared to the structurally homogeneous amorphous material. We attribute this newly identified magnetic phase to the glass-glass interfaces, where the decreased atomic density leads to enhanced exchange interactions following the Bethe-Slater formalism.

MM 17.78 Mon 17:00 Poster B

Kinetic processes in copper bi- and tricrystals — •Isabelle Binkowski[1], Henning Edelhoff[1], Jörn Leuthold[1], Matthias Wegner[1], Martin Peterlechner[1], Shashank Shekhar[2], Alexander King[3], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]Indian Institute of Technology Kanpur Kalyanpur, Kanpur - 208 016 — [3]The Ames Laboratory, 311 TASF, Iowa State University Ames, IA 50011-3020

Grain boundaries (GBs) and their junctions often define properties of polycrystals and have an influence on diffusion and plastic behavior. Because of the high density of GBs included in polycrystalline materials and especially nanocrystalline materials, investigation of kinetic processes in this type of defect are of fundamental interest. Heading towards nanostructured materials one has to focus also on triple junctions (TJs) since their volume fraction and correlative their influence on materials' properties rise. In the present investigation, a near special $\Sigma(5):\Sigma(5):\Sigma(25)$ copper tricrystal is utilized to examine the properties of a TJ with defined orientation of grains and misorientation across the GBs. The mass transport properties of the tricrystal are investigated using the radiotracer method. The kinetics of out-diffusion from the TJ into the neighboring GBs are measured by preparing proper bicrystalline samples. Additionally, tensile tests including plastic deformation of several percent are performed and the digital image correlation technique is applied to measure the strain fields in the immediate vicinity of GBs and TJs.

MM 17.79 Mon 17:00 Poster B

Reactive Diffusion and Stress in Core-Shell Nanostructures — Zoltan Erdelyi[1], Christian Buchholz[2], and •Guido Schmitz[2] — [1]Department of Solid State Physics, University of Debrecen, Hungary — [2]Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

In comparison to planar multilayers, core-shell and hollow nanospheres show remarkably different kinetics of solid state reaction, since much higher levels of reaction-induced stress can develop in closed spherical geometries. We present a completely analytical model to calculate the development and anisotropic plastic relaxation of stress during reactive diffusion in spherical geometry. The complex model can be considered as a generalization of Stephenson's model (Acta Metallurgica 1988;

36:2663). It is demonstrated that growth rates in nanometric spherical diffusion couples may switch from fast Darken interdiffusion to slow Nernst-Planck interdiffusion regime in dependence of layer stacking sequence. In triple layers A/B/A, the reaction rate at both interfaces may become remarkably different as has been indeed observed experimentally (Schmitz et al. Acta Mat. 2009; 57:2673) by atom probe tomography.

MM 17.80 Mon 17:00 Poster B

Study of the EFGs at both M- and A-sites in Zr_2InC and Hf_2InC using γ-γ angular correlation spectroscopy — •Daniel Jürgens[1], Michael Uhrmacher[1], Ulrich Vetter[1], Hans Hofsäss[1], Jose Mestnik-Filho[2], and Michel W. Barsoum[3] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil — [3]Dep. Mat. Science and Eng. Drexel University, Philadelphia, PA 19104, USA

The compounds Zr_2InC and Hf_2InC belong to the class of MAX phases, which are known for their metallic and ceramic characteristics. Due to their unusual set of properties, these phases have been studied intensively in recent years with the aim to find new high-performance materials. Since most applied techniques only allow a macroscopic insight, the perturbed angular correlation (PAC) was used to determine the local environment of inserted probes on atomic scale. Radioactive ^{111}In and ^{181}Hf ions were implanted into the samples to measure characteristic electric field gradients, EFGs, at a certain site. The A-site EFG was investigated by using the ^{111}In isotope and the M-site by ^{181}Hf probes. In this study we report on the different annealing behaviors of In- and Hf-probes in Zr_2InC and Hf_2InC. We show that the A-site EFG strengths are nearly identical ($\nu_Q \approx 350$ MHz), while the EFGs for the M-site are unequal. We compare the experimental results with predictions from density functional theory calculations and give reasons why the A- and M-site EFGs are in such a way dissimilar.

MM 17.81 Mon 17:00 Poster B

The effect of the stacking sequence on the EFG in the MAX phase systems Ti-Al-X (X = C, N) — •Daniel Jürgens[1], Michael Uhrmacher[1], Ulrich Vetter[1], Hans Hofsäss[1], Jose Mestnik-Filho[2], and Michel W. Barsoum[3] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil — [3]Dep. Mat. Science and Eng. Drexel University, Philadelphia, PA 19104, USA

$M_{n+1}AX_n$ phases are nanolaminated layered ternary compounds and show both metallic and ceramic characteristics. These materials show an unusual set of properties and are therefore potential candidates e.g. for high-temperature applications. Most MAX phases belong to the 211 subclass (i.e. $n = 1$) and are made up of M_6X octahedra layers, which are separated from each other by one inserted A-layer. Only a few compounds exist with 312 (and 413) stoichiometry, where two (three) M_6X layers are embedded between two A-layers. The Ti-Al-C system is one among the few which can be synthesized in the 211 and 312 structure. For the Ti-Al-N system, the only stable compounds belong to the 211 and 413 classes.
By means of perturbed angular correlation (PAC), we measured the electric field gradients (EFGs) at the Al-site in these compounds. We could observe that the strength of the EFGs differ significantly between the different stacking sequences of the same system. In this contribution we show the experimental results and discuss the potential reasons for this effect.

MM 17.82 Mon 17:00 Poster B

2D quench calculations for FAIR Super-FRS dipole — •Piotr Szwangruber[1,2], Eric Floch[2], Thomas Weiland[1], and Oliver Boine-Frankenheim[1] — [1]Technische Universität Darmstadt, Institut für Theorie Elektromagnetischer Felder, Darmstadt, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany

The Super Fragment Separator (Super-FRS) will be a part of the Facility for Antiproton and Ion Research (FAIR) placed in Darmstadt, Germany. Super-FRS will have superferric superconducting magnets working in liquid helium. Superconducting magnets need to be protected against quench (unwanted transition from superconducting to normal conducting state). To foresee the temperature distribution and voltage increase during a quench and to choose the best magnet protection system one needs to do the quench calculations before the first test of the magnet prototype.

This work presents a comparison between 2D quench calculations done on FAIR Super-FRS dipole with two different quench programs. The first was developed in GSI. It uses finite difference method and it is based on the heat equation. The second was a commercial FEM (FInite Element Method) software Opera 3D with the quench module. Obtained results are in good accordance between those programs.

MM 17.83 Mon 17:00 Poster B

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

The excellent physical properties of graphene make it a promising material for many scientific applications. The high electron mobility [1] and the relatively long spin lifetime [2] leading in spin diffusion lengths λ up to 2 microns [3], which make it a very interesting candidate for spintronics. By using of turbostratic graphene (TG), a multilayer of electronically decoupled graphene layers, one can overcome limits of λ like interaction between substrate and graphene as well as intrinsic corrugation in graphene sheets. TG combines the exciting properties of graphene with the higher robustness to environmental influences and the absence of inner corrugations of a microstructured material [4]. We present here successful spin injection from ferromagnetic electrodes into TG discs (in non-local spin valve configuration [3]) as well as transport properties of TG. [1] A. K. Geim et al., Nature Materials 6, 183 (2007), Science 324, 1530 (2009). [2] Hernando et al., Phys. Rev. B 74, 155426 (2006). [3] N. Tombros et al., Nature 448, 571 (2007). [4] M. Orlita et al., Phys. Rev. Lett. 101, 267601 (2008).

MM 17.84 Mon 17:00 Poster B

Ab initio-based mean field theory of site occupation in binary sigma phases — •Evgeniya Kabliman[1], Andrei V. Ruban[2], Oleg E. Peil[3], Peter Blaha[1], Karlheinz Schwarz[1], and Börje Johansson[2] — [1]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria — [2]Department of Materials Science and Engineering, Applied Material Physics, Royal Institute of Technology, Brinellvägen 23, SE-100 44 Stockholm, Sweden — [3]I. Institut of Theoretical Physics, Hamburg University, Jungiusstrasse 9, 20355 Hamburg, Germany

In present work we study the atomic site distribution in binary sigma-phases, which are found in many industrial alloys and usually lead to a destructive effect on the mechanical properties of these alloys. For this purpose we have proposed a simple and powerful approach to calculate the site occupation numbers as function of temperature and composition [1,2]. It is based on the single-site mean-field description of the free energy, where the total energy is expanded in terms of on-site effective cluster interactions, which are calculated as relative chemical potentials. The suggested method has been successfully applied to the Fe-Cr, Co-Cr, Re-W and Fe-V sigma-phases.

[1] E. Kabliman, P. Blaha, K. Schwarz, A. V. Ruban, B. Johansson, Phys. Rev. B 83, 092201 (2011); [2] E. Kabliman, P. Blaha, K. Schwarz, O. Peil, A. V. Ruban, B. Johansson, Phys. Rev. B 84, 184206 (2011).

MM 17.85 Mon 17:00 Poster B

Ab-initio calculations of mechanical properties of TaxMo1-xN — •Khellil Bouamama — Laboratoire d'optoélectronique et composants, Université Ferhat Abbas, 19000 Sétif, Algeria

First-principles pseudopotential calculations of the lattice constants and of the mechanical properties for TaxMo1-xN alloys with B1-rocksalt structure were carried out. These calculations were performed using density functional perturbation theory (DFPT) within the virtual crystal approximation (VCA) for the disordered alloys and the supercell method (SC) for the ordered alloys. For the exchange-correlation potential the generalized gradient methods (GGA)is used. It is found that the addition of Mo induces a decisively ductile character in the clearly brittle TaN.

Keywords: Ab-initio, VCA, DFPT, nitride materials, elasticity

MM 17.86 Mon 17:00 Poster B

On the conductivity and chemical stability of lithium con-

ducting glass ceramics (LICGC): Application in next generation batteries? — •Pascal Hartmann[1], Marisa Reich[2], Thomas Leichtweiss[1], Meike Schneider[2], Wolfgang Schmidbauer[2], and Jürgen Janek[1] — [1]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]SCHOTT AG, Corporate Research and Technology Development, 55014 Mainz, Germany

To fullfill future requirements in terms of electrical energy storage highly reactive materials will be used as active electrode components in the so-called next generation batteries. Most of the known liquid organic electrolytes decompose in contact with these materials making them not applicable. Therefore much effort has been spent to develop inorganic solid lithium electrolytes in order to protect the organic liquids or even completely replace them. One class of materials are glass ceramics. Especially the system $Li_{1+x}AlM(PO_4)_3$ (M = Ge, Ti,...) was intensively studied and it was claimed that these materials show a lithium ion conductivity of more than 1 mS/cm and that Ti-free samples, in addition, show good chemical stability upon reduction reactions. In this work we investigated glass ceramic materials with different ratios of Ge and Ti using electron microscopy, impedance spectroscopy, and low current polarization techniques. We show that there is a trend in terms of ionic conductivity, electronic conductivity and chemical stability upon the contents of Ge and Ti. These studies help to identify suitable material compositions to fulfill the requirements for long term stable and safe next generation batteries.

MM 17.87 Mon 17:00 Poster B

A new 2D-ACAR spectrometer at the NEPOMUC positron facility — •Hubert Ceeh[1], Josef Weber[1], Christoph Hugenschmidt[1,2], Michael Leitner[3], and Peter Böni[1] — [1]Technische Universität München E21, Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz, Garching, Germany — [3]Technische Universität München E13, Garching, Germany

The 2D-ACAR (Angular Correlation of Annihilation Radiation) technique is a well suited method for the investigation of the electronic structure, in particular the fermiology of correlated systems. Measuring the two dimensional projection of the two-photon-momentum-distribution of the annihilation radiation the three dimensional electron momentum distribution can be calculated via tomographic reconstruction. A new 2D-ACAR spectrometer is currently being installed at the NEPOMUC facility at the research reactor in Garching. In the setup, the positrons from a 50 mCi ^{22}Na source are guided onto the sample by an axial magnetic field created by a normal conducting electromagnet. The use of especially developed soft iron pole caps, guarantees a homogeneous magnetic field with a magnetic flux density > 1.2 T while allowing axial access to the sample- and positioning stage. The sample stage itself can be cooled by a standard cryo-cooler to temperatures below 30 K in order to reduce the smearing of the angular resolution by the positron momentum. The key features of the new spectrometer are presented. In addition, first results of measurements on a intermetalic Heussler crystal are discussed and compared with first principle band structure calculations.

MM 17.88 Mon 17:00 Poster B

The effect of grain size and grain boundaries on the mechanical behaviour of MAX phases — •Thilo Seliger[1], Cynthia Volkert[1], Christoph Brüsewitz[2], Hans Hofsäss[2], and Michael Uhrmacher[2] — [1]Institut für Materialphysik, Universität Göttingen, D-37073 Göttingen — [2]II. Physikalisches Institut, Universität Göttingen, D-37073 Göttingen

It is well known that the MAX phases (layered ternary carbides and nitrides) have unusual mechanical properties. They exhibit features from both metals (machinable, damage tolerant, good thermal and electrical conductivities) and from ceramics (high stiffness and low thermal expansion). This is attributed to the fact that dislocations only move on a single set of parallel planes, which results in kinking and shear band formation during deformation. It has been observed that the formation of kinks and shear bands is influenced by the grain size, leading to an increase in strength with decreasing grain size. We seek to take advantage of the grain size dependent strength and the damage tolerance of the MAX phases to explore the possibility of designing nanocrystalline MAX phases with both high strength and high ductility. We investigate the effect of grain size and individual grain boundaries on the nanoindentation response of Ti-based bulk MAX phases. A combination of EBSD to determine grain orientations, focused ion beam to mark specific locations and Berkovich nanoindentation have been used. The relation between local mechanical properties and local microstructure will be presented and discussed and used to develop guidelines for optimum grain sizes and textures.

MM 17.89 Mon 17:00 Poster B

Advanced EBSD/EDS integration for efficient and modern materials characterization — Daniel Goran, Laurie Palasse, and •Thomas Schwager — Bruker Nano GmbH, Schwarzschildstrasse 12, 12489, Berlin, Germany

Recent software and hardware developments have greatly increased the speed at which simultane-ous Electron BackScatter Diffraction (EBSD) and Energy Dispersive X-Ray Spectroscopy (EDS) mapping can be done. We will demonstrate that new developments have transformed the combina-tion of these techniques into a powerful tool for characterizing multiphase materials with improved efficiency and data quality, introducing new ways of using the two complementary techniques to ensure data integrity.

It is well known that the information delivered either by EBSD or by EDS alone is not enough to successfully distinguish the different phases present, like for phases creating similar patterns or sim-ilar chemical composition. Typical examples are quartz and cristobalite, rutile and magnetite.. The new approach consists of simultaneously acquiring an EBSP and a complete EDS spectrum for each point in the map (up to 500 points/sec), then a two-step online/offline analysis method can be used to automatically discriminate phases creating similar patterns using the quantified EDS results to decide or narrow down the phase in each point, finding the correct crystallographic orientation for that particular point. Moreover, if one or more unknown/unexpected phases are present, the EDS information can be used for offline phase identification (up to 54000 points/sec).