# MM 18: Poster Session

Time: Monday 18:00–20:00 Location: P4

MM 18.1 Mon 18:00 P4

**Microstructural Evolution of Nanoporous Gold During Coarsening** — •Markus Ziehmer[1], Kaixiong Hu[1], Ke Wang[2], Jürgen Markmann[1,2], and Erica Lilleodden[1] — [1]Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Geesthacht, Germany — [2]Hamburg University of Technology, Institute of Materials Physics and Technology, Hamburg, Germany

Nanoporous gold (npg) has gained much interest in the past decade for being a promising candidate for technical applications. The fact that the mean structural sizes can be easily adjusted makes it even more interesting as a functional material. This requires a comprehensive understanding of the microstructure evolution.

Presently, scaling laws are often used to predict the mechanical performance of npg that rely on global parameters like the solid volume fraction. However, these measures are obviously insufficient to take into account the complex microstructure of npg that ultimately governs the behaviour. Such scaling laws implicitly assume some kind of self-similar evolution during coarsening with regard to morphology and topology. Furthermore, the evolution of the crystallographic orientations of the ligament network is mostly disregarded.

In our work, we apply high-resolution FIB tomography on npg samples with different structural sizes together with EBSD measurements for an investigation on the microstructure evolution of npg.

The results are discussed within the context of the validity of self-similar approximation inherent in scaling laws.

MM 18.2 Mon 18:00 P4

**Thin-film cathodes for application in lithium ion batteries** — •Martin Fiedler[1], Frank Berkemeier[1], and Guido Schmitz[2] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institut für Materialwissenschaften, Universität Stuttgart, Heisenbergstr. 3, 70569 Stuttgart

Lithium Cobalt Oxide (LCO) and Lithium Iron Phosphate (LFP) powder material is commonly used in commercial lithium ion batteries. In this work, thin LCO and LFP films between 200 and 5500 nm in thickness are prepared by magnetron sputtering. After deposition, the layers are characterized by X-ray diffraction, transmission electron microscopy, and electrochemical techniques like cyclic voltammetry and chronopotentiometry. The influence of a negative substrate bias during sputter-deposition and of post annealing between 400 and 700°C is investigated, and it is found that the electrochemical performance of the layers significantly depends on both parameters. The preparation of films under optimized conditions gives smooth thin-film cathodes, with a maximum thickness of 5500 nm and a lateral size of 45 $cm^2$. In case of LCO, this results in a lithium storage capacity up to 17 mAh. Despite their large thickness, the cathodes are mechanically stable and allow the investigation of transport kinetics without being influenced by interface effects. Moreover, they open the possibility to be used in technical lithium ion batteries, as substitutes for conventional powder cathodes.

MM 18.3 Mon 18:00 P4

**Materials for all solid-state lithium-ion batteries** — •Susann Nowak[1], Frank Berkemeier[2] und Guido Schmitz[1] — [1]Institut für Materialwissenschaften, Heisenbergstr. 3, 70569 Stuttgart — [2]Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

All solid-state batteries present a very interesting model system for studies on kinetics and thermodynamics in lithium-ion batteries, but are particularly demanding in the specifications needed for the utilization of materials as their components, for example they have to show a very low surface roughness. In the current poster we present the fabrication and characterization of different materials, which can be used in an all solid-state batteries. The properties of lithium iron phosphate, lithium phosphorous oxynitride and tin are shown. Fabrication is carried out by ion beam sputtering and in the case of lithium iron phosphate post annealing under argon atmosphere. Characterization is carried out via electrochemical methods (chrono potentiometry and cyclic voltammetry), charge state depending x-ray diffraction (XRD), and transmission electron microscopy (TEM). An outlook on measurements on a complete all solid-state system is given.

MM 18.4 Mon 18:00 P4

**Sputter-deposited Thin-film Lithium Ion Batteries** — •Frank Berkemeier, Yaser Hamedi, and Fabian Inkmann — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Electrochemical-active thin-film materials are deposited by sputter-deposition technique, with the aim to prepare an all-solid state thin-film lithium-ion battery. For this purpose silicon and tin are used as anode materials, while lithium cobalt oxide and lithium iron phosphate serve as cathodes. As an ion-conducting phase, thin-films of lithium phosphorous oxynitride (LiPON) are deposited. Via this setup, thin-film stacks with an overall thickness of less than 1$\mu$m are prepared, which are characterized by electrochemical techniques like impedance spectroscopy and cyclic voltammetry, as well as by transmission electron microscopy. It is shown that most of the thin-film cells show a reasonable charge-discharge behaviour, as well as a promissing cycling stability. Moreover it is demonstrated that by triggering a reaction between LiPON and a metallic layer like silver or magnesium, an interface reaction layer is formed that is capable to reversibly intercalate/deintercalate lithium. The structure and formation of this reaction layer is studied, and it is shown that in future thin-film cells this layer opens the possibility to substitute conventional thin-film cathodes – with the aim to increase the energy density and to decrease the internal resistance of the cells.

MM 18.5 Mon 18:00 P4

**Nanostructured black silicon as anode 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, Germany — [2]Martin-Luther-University Halle-Wittenberg, Halle, Germany

It has been known for some time past 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. 320%) during lithiation/delithiation, resulting in mechanical disintegration of electrode and rapid capacity fading. Therefore, relaxation of the stress caused by the expansion and contraction of Li-Si alloy materials is important to obtain a good cycleability. Furthermore, the formation of solid electrolyte interphase (SEI) induced by decomposition of electrolyte hinders lithium ion movement during the Li-Si alloying/de-alloying, resulting in poor capacity retention upon cycles. In this study, we prepared well-ordered nanostructured black silicon arrays (nb-Si) on silicon substrate by gas chopping technique. The electrochemical properties of the nb-Si electrode were systematically investigated. The material characteristics have been analyzed by CV, SEM and TEM. The performance of nb-Si electrode has been examined by galvanostatic charge/discharge cycling. In order to understand the correlation between surface condition and Li-Si alloying, we have investigated the surface composition of nb-Si electrode before and after pretreatment by means of high resolution XPS as well

MM 18.6 Mon 18:00 P4

**In-situ TEM studies of nanostructured Mg based hydrides at elevated hydrogen pressures of 1 bar** — •Alexander Surrey[1,2], Ludwig Schultz[1,2], and Bernd Rellinghaus[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institut fur Festkörperphysik, D-01062 Dresden, Germany

In the search of materials that are potentially applicable as solid-state hydrogen storage materials in the mobile and stationary sector, $MgH_2$ is considered one of the most promising hydrides due to both its relatively high gravimetric storage density of 7.7 wt.-% and its high abundance. However, the thermodynamic and kinetic properties of intrinsic $MgH_2$ impede a practical application. Here, nanostructured hydrides have been shown to reveal improved (de)hydrogenation properties. During structural characterization utilizing conventional TEM, however, $MgH_2$ degrades fast upon the irradiation with the imaging electron beam due to radiolysis in vacuum and as a consequence, the hydride phase cannot be studied at highest resolution. To overcome this problem we explore the possibility to investigate Mg based hydrides by in-situ TEM at elevated $H_2$ pressures (1 bar) and

temperatures (up to 300°C) using a so called nanoreactor that was recently developed by Henny Zandbergen at the TU Delft. This allows to study the dehydrogenation as well as the hydrogenation reaction at the nanoscale under working conditions. We present multi-slice HRTEM contrast simulations to show the possibilities and limitations of this new nanoreactor. Such simulations may be valuable to pre-evaluate future experiments.

MM 18.7 Mon 18:00 P4

**Influence of temperature on hydrogen induced surface modification on Gd(0001) islands** — •Samuel Königshofen, Sara Wanjelik, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

The adsorption of hydrogen on metal surfaces is of great interest in fundamental research and also applied science due to its importance for technology and material science. Although there has been research for many years, the subsequent hydride formation and especially their initial behavior is not completely understood yet. Here we present measurements, carried out by scanning tunneling microscopy, on gadolinium islands of 100-400 nm size and a few nanometers in height. The islands are grown on a W(110) surface. The initial stage of hydride formation and the localization of its occurrence will be of special interest. Further, the appearance and change of the hydrides due to heating of the sample has been observed. The steps of the temperature variation are in the range of a few hundred kelvin starting at room temperature. Additionally, the time dependence of the formation will be discussed. The known occurrence of disc-like island and formation of ramps on Gd thin films due to hydrogen adsorption will be compared to the investigated hydride characteristics of Gd islands.

MM 18.8 Mon 18:00 P4

**Preparation of a Ta(110) surface for hydrogen absorption** — •Sebastian Schleicher, Sara Wanjelik, and Mathias Getzlaff — Institut für Angewandte Physik, Universität Düsseldorf, Deutschland

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. In our study we investigate hydrogen on adsorption and absorption in a Ta(110) crystal which requires careful cleaning as preparation for any measurement on the Tantalum surface. The cleaning procedures include heating up to 2900°C, annealing in an oxygen atmosphere and sputtering with a sputter ion source to remove impurities. The subsequently observed superstructure remains unaffected and may show a reconstructed pattern of a clean Tantalum surface. Measurements are performed by means of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) under ultrahigh vacuum conditions.

MM 18.9 Mon 18:00 P4

**A new additive-assisted synthesis route and electrochemical properties of olivine LiCoPO4** — •Christoph Neef[1], Hans-Peter Meyer[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg — [2]Institut für Geowissenschaften, Universität Heidelberg, D-69120 Heidelberg

Olivine LiCoPO4 micro- and nanocrystals were synthesized applying a two-step process starting by hydrothermal growth of non-olivine LiCoPO4-tetra which then is transformed to the olivine phase at high temperatures. By adding various organic additives such as sugars, acids, organic solvents, and ammonia compounds in step 1, the shape, size, and tendency to agglomeration of the obtained particles is investigated. This yields a variety in particle morphologies. Galvanostatic cycling and impedance spectroscopy show strong differences in the electrochemical performance of the different materials. In particular, the rate capability strongly depends on the morphology as well as aging effects due to electrolyte decomposition, the latter being typical for high voltage materials like LiCoPO4.

MM 18.10 Mon 18:00 P4

**Pathway to mechanically stable magnetocaloric cycling materials** — •Alexander Funk[1,3], Anja Waske[1], Maria Krautz[2], Bruno Weise[1,3], Konstantin Skokov[4], and Jürgen Eckert[1] — [1]Institute for Complex Materials, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Institute for Metallic Materials, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Institute for Material Science, TU Dresden, Helmholtzstraße 7, 01069 Dresden, Germany — [4]Material Science, TU Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

Magnetocaloric materials could one day be the basis of a new magnetic cooling concept for consumer use, replacing conventional refrigeration technology. The research in magnetocalorics focused on the discovery and development of materials with large or giant magnetocaloric effects (MCE) over the last few decades. Such alloys [1, 2] show a 1st order phase transition, with a simultaneous structural and magnetic change. Therefore bulk MCE-materials often show mechanical instability during magnetic field cycling. Here, we present an approach to produce high quality MCE-materials which overcomes these problems. Results on magnetocaloric properties were obtained by magnetometry and direct ΔTad measurements. The materials structure and mechanical stability after cycling (e.g. crack development) were observed by X-Ray computed tomography and SEM.

References:
[1] V.K. Pecharsky et al., Phys. Rev. Lett. 78, 4494 (1997)
[2] D.T. Cam Thanh et al., J. Appl. Phys. 99, 08Q107 (2006)

MM 18.11 Mon 18:00 P4

**Graphitization and interface bonding in carbon-bonded alumina ceramics** — •Torsten Weissbach, Masud Alam, Christian Röder, Lilit Amirkhanyan, and Jens Kortus — Institut f. Theoretische Physik, TU Bergakademie Freiberg, 09596 Freiberg

Refractory ceramics reinforced with carbon [1] show an improved resistance to thermal shock, due to the high thermal conductivity of carbon. We present Raman scattering results [2] on these compound materials, which show that carbon is forming graphitic clusters at the surface of the ceramic and that allow for determination of the cluster size of the graphite fractions. In addition, density functional calculations were performed to model the interface between alumina and graphite. By applying an empirical correction for the dispersion interactions [3], we study the different contributions to bond formation in several possible interface geometries. The formation of strong polar bonds is only found at oxygen sites on the surface.

[1] Markus Emmel et al., Ceramics International (2012)
[2] Christian Röder et al., Journal of Raman Spectroscopy, accepted
[3] Stefan Grimme, Journal of Computational Chemistry (2006)

MM 18.12 Mon 18:00 P4

**Light-driven rotation of chiral, screw-like microstructures in a fluidic environment** — •Lindsey JE Anderson[1], Silke Kirchner[1], Debora Schamel[2], Peer Fischer[2], Theobald Lomüller[1], and Jochen Feldmann[1] — [1]Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universtität München, Amalienstr. 54 80799 Munich, Germany — [2]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3 70569 Stuttgart, Germany

Propulsion of nano and micron-scale objects controlled by a remote stimulus is of great interest for creating machines and sensors in microfluidic environments. We study the influence of light on chiral, screw-like silica particles which are fabricated with glancing angle deposition. In an optical trap, these structures orient along the optical axis and radiation pressure causes them to rotate with a frequency that is proportional to the laser power. The rotation of these structures makes them candidates for artificial propellers, with a geometry that allows for the possibility of easily permeating biological membranes. Because of the highly controllable fabrication process, it is possible to design hybrid metallic propellers with this chiral structure and study how plasmonic interactions influence their functionality.

MM 18.13 Mon 18:00 P4

**Phase-field simulation of interdiffusion-limited coarsening in Ni-base superalloys under applied loads** — •Leslie Mushongera, Micheal Fleck, Julia Kundin, and Heike Emmerich — University of Bayreuth

We study microstructure evolution in Ni-base superalloys under a uniaxial strain applied along a cubic axis. It is observed that the gamma prime precipitates age from quasi-cuboids to rafts aligned along the <100> direction. It is observed that slow diffusing elements particularly, the refractory element Re, play a major role in reducing the rate of rafting. Re additions substantially reduce the rate of rafting by enforcing some gamma prime precipitates to keep the energy minimizing quasi-cuboidal configuration while on the other hand, hindering the elongation of rafts. In addition, a numerical technique to characterize the coarsening kinetics of microstructures with self-dissimilar gamma prime precipitates is presented.

MM 18.14 Mon 18:00 P4

**Continuum modelling of grain boundary wetting** — •Venkata Sai Pavan Kumar Bhogireddy[1], Fabian Twiste[1], Chi-Dzu Nguyen[1], Claas Hüter[1], Robert Spatschek[1], Jörg Neugebauer[1], Alain Karma[2], and Efim Brener[3] — [1]Max Planck Institut für Eisenforschung, D-40237, Düsseldorf, Germany — [2]Physics Department, Northeastern University, Boston, 02115, USA — [3]Peter Grünberg Institut, Forschungszentrum Jülich, D-52425, Jülich, Germany

Grain boundary (GB) premelting describes the appearance of thin nanometric melt layers along grain boundaries already below the bulk melting point, which can lead to dramatic material failure. Amplitude equations modelling shows that the premelting transition depends on the misorientation between the grains due to short range interactions between the adjacent crystals. In the absence of a misorientation a translational shift between the grains can still lead to periodic modulations of the interaction potential in the spirit of gamma surfaces, hence linking mesoscopic continuum models to atomistic descriptions. The tail of these interactions can be predicted analytically, and the results are compared to numerical results, which are also valid at shorter distances. Furthermore, we investigate the possibility of a conventional phase field model based on the multi-obstacle potential to capture the premelting transition.

Apart from these static situations we also study the penetration of a melt front along the GB in an overheated crystal, taking into account the aforementioned short ranged interactions. We find that the penetration velocity is strongly influenced by the nanoscopic interactions.

MM 18.15 Mon 18:00 P4

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

MnAs is a promising ferromagnetic material for magnetoelectronic devices, in particular as nano-scaled clusters, providing a great tunability concerning the shape and position. We investigate hexagonal MnAs clusters separated by a metal. For doing a simulation of this problem we developed an effective potential for MnAs by means of the Force Matching Method. The resulting potential, fitted to ab initio data, describes the substrate of our deposition simulation. The interaction between substrate atoms and the deposition atoms (here gold) is also done in the scope of Force Matching. Both interaction potentials are based on the Embedding Atom Method, which turned out to be a suitable model for the materials at hand as we prove with some validation tests.

MM 18.16 Mon 18:00 P4

**Modeling phase transformations in binary alloys for eutectic systems** — •Muhammad Ajmal Choudhary[1], Julia Kundin[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth. — [2]Institut für Angewandte Physik, Universität Tübingen, D-72076 Tübingen.

Phase-field crystal (PFC) modeling has emerged as a promising technique to address the crystal growth phenomena on atomistic length and diffusive time scales. We use a 2D PFC model for a binary alloy system based on Elder et al. [Phy. Rev. B 75, 064107 (2007)] to investigate the size effects on the equilibrium properties of the liquid-solid interface. We analyze the equilibrium properties of liquid-solid interface by stabilizing the circular solid crystal of various radii in the surrounding liquid phase and the liquid droplets of various radii in the solid phase in a finite system size. In particular, we propose the method of determining interfacial energies for a curved liquid-solid interface as function of radius by integrating the grand potential density over the simulation domain. Furthermore, we also derive the free energy barriers for the nucleation and compare the results with the prediction based on the classical nucleation theory.

MM 18.17 Mon 18:00 P4

**Effect of surfaces and interfaces on elastic properties of transition metals studied by DFT and EAM** — •Tobias Klöffel[1], Erik Bitzek[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Department of Materials Science and Engineering, WW 1: General Materials Properties, FAU Erlangen-Nürnberg

Experimental studies show that defect-free metallic nanowires exhibit different elastic properties compared to their bulk counterparts. Atomistic calculations with embedded atom method (EAM) potentials show the same trend, however, at much smaller wire diameters. In addition, recent studies indicate that even nanowires with relative large diameter of about 200 nm to 1000 nm might posses a lower Young's modulus, if they incorporate hundreds of twin boundaries (TBs) parallel to the wire axis.

We present first results of systematic atomistic calculations, searching for a possible source of this yet unknown effect, which could be responsible for a decreased Young's modulus $E$. We first calculated $E$ for a defect-free bulk cell and compared the results to a cell that included TBs parallel to the direction of the Young's modulus using DFT. We also compared the interface-stress calculated by DFT and EAM to the surface-stresses, which are known to influence the elastic properties of materials. In a second step, we compared the elastic properties of model wires of different sizes with and without TBs using EAM potentials. First results will be discussed and compared to experimental findings.

MM 18.18 Mon 18:00 P4

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

The oscillation behaviour of nanomechanical resonators in the form of doubly clamped beams and clamped membranes is investigated by molecular dynamics simulations. After setting up the initial structure, the end points of the beams or the outer border of the membranes, respectively, 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 structures. Besides varying the size of the structures, the effects of temperature, external stretching fields, cavities and crystal faults are explored. The results show a decrease of the oscillation frequencies and an increase of the damping coefficient with rising temperature, a strong increase of the frequencies with external stress (stretching), a decrease of frequencies with size and an increase of the damping coefficient when adding cavities to the structures. It is also possible to observe the dissipation of energy from the collective oscillation of the structures into thermal energy of the degrees of freedom of the constituting atoms. Different materials (e.g. $Si$, $Si_3N_4$ and $NiTi$ memory alloys) are explored as well. In order to explore quantum effects in the low temperature regime path integral Monte Carlo simulations are performed.

MM 18.19 Mon 18:00 P4

**Heat capacity of $Al_3FeSi_2$: Quasiharmonic approximation versus Neumann-Kopp rule and measurement** — •Lilit Amirkhanyan[1], Torsten Weissbach[1], Thomas Gruber[1], Olga Fabrichnaya[2], Tilo Zienert[2], and Jens Kortus[1] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09596 Freiberg, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Straße 5, D-09595 Freiberg, Germany

Thermodynamic databases are an important tool for the simulation of solid state reactions and phase diagrams. In cases when the thermodynamic data are not available for a certain compound, they are calculated in approximation from elemental data (Neumann-Kopp rule [1]). Here we compare experimental DSC data with the Neumann-Kopp rule and first-principles calculations based on DFT and the quasiharmonic approximation. The compound in question is the $\tau_4$-AlFeSi phase, a ternary light-metal alloy from the Aluminium-rich side of the system. We show that the DFT-QHA calculations are in good accord with the measured heat capacity ($c_p$), while the N-K rule suffers several shortcomings.

[1] J. Leitner et al., Thermochimica Acta, 2010

MM 18.20 Mon 18:00 P4

**Temperature dependence of the elastic constants of W: An ab-initio study** — •Thomas Dengg[1,2], Jürgen Spitaler[1], Lorenz Romaner[1], and Peter Puschnig[2] — [1]Materials Center Leoben Forschung GmbH — [2]Karl-Franzens-Universität Graz, Institut für Physik

Two different ab-initio approaches for calculating the temperature dependence of the elastic constants of W are investigated. On the one hand the influence of temperature is taken into account only through the volume expansion. Here, thermal expansion can either be taken from experiment or determined theoretically within the quasiharmonic

approximation. On the other hand the temperature dependence can explicitly be determined by calculating the free energy as a function of strain. To this end, the phonon density of states is calculated for a set of strained structures. The results from both approaches are compared with each other and it is assessed how they perform in terms of computational effort and accuracy and last but not least how well they agree with experimental values.

MM 18.21 Mon 18:00 P4

**The $F$ Center in Lithium Fluoride revisited: comparison of solid-state physics and quantum-chemistry approaches** — •Ferenc Karsai[1], Paul Tiwald[1], Joachim Burgdörfer[1], Peter Blaha[1], Ludger Wirtz[2], Robert Laskowski[1], Fabien Tran[1], David Koller[1], and Stefanie Gräfe[1] — [1]Vienna University of Technology, Vienna, Austria — [2]University of Luxembourg, Luxembourg, Luxembourg

The F-type color-center in LiF is an old prototype problem where an electron is trapped at a vacant anion site. In an intuitive picture the defect electron can be approximately described as a particle in the box. We present a comparison of the physicist's approach (periodic supercell-approach with various DFT-functionals, GW and Bethe-Salpeter methods) and the quantum-chemist's approach (embedded-cluster approach with wave-function methods such as CASPT2). In both cases, we observe strong excitonic effects due to the strong localization of the defect in agreement with the simple particle in box picture. We also find that the calculated absorption spectra from both approaches are in unprecedented agreement with experiment.

MM 18.22 Mon 18:00 P4

**On low-energy electronic excitations in the $Ti_{1-x}Al_xN$-system** — •Simon Lamowski, Torsten Weissbach, and Jens Kortus — TU Bergakademie Freiberg, Institut für TheoretischePhysik, Leipziger Straße 23, 09599 Freiberg, Germany

Layered structures of $Ti_{1-x}Al_xN$ were experimentally characterized by electron energy-loss spectroscopy (EELS) scanned along a direction perpendicular to the interface. By means of ab initio Density Functional Theory (DFT) calculations using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the Elk code [1] we investigated structural and electronic factors which influence the EELS up to an energy-loss of 60 eV.

The stability of different structures are calculated with a cluster expansion technique as implemented in the ATAT program package [2].

Further, we go beyond standard DFT by using time-dependent DFT with the bootstrap kernel [3]. This enables us to use time-dependent DFT in calculation for crystalline solids.

[1] Dewhurst K, et al. Elk. Version: 2.2.09 Available from: http://elk.sourceforge.net/

[2] van de Walle A, et al. ATAT. Version: 2.71 Available from: http://www.brown.edu/Departments/Engineering/Labs/avdw/atat/

[3] Sharma S, et al. Physical Review Letters; 2011; 107(18): 186401

MM 18.23 Mon 18:00 P4

**Atomistic modelling of phase transitions in Ti-Ta high-temperature shape memory alloys** — •Tanmoy Chakraborty, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Shape memory alloys (SMAs) exhibit unique properties that are used in applications such as couplings, sensors or actuators in automobile industry, aviation and in other technological areas. To extend their range of applicability, it is of particular interest to develop SMAs that can be used at high temperatures (HTSMA), with a martensitic transformation temperature well above 373K. Promising results for a novel HTSMA have been found for the Ti-Ta system. Experimentally it has been observed that a large Ta concentration stabilizes the shape memory effect due to supressing the formation of the detrimental $\omega$ phase. But an increasing Ta content also leads to a reduction of the martensitic transformation temperature.

In our study, we apply density functional theory (DFT) calculations to investigate the stability of the involved phases ($\alpha$", $\beta$, $\omega$) as a function of the Ta concentration. To determine the mechanical and dynamical stability of the different phases, we calculate elastic constants and phonon spectra. Furthermore, the phonon density of states is used to include vibrational contributions to the free energy which allows us to compare the relative stability of the different phases as a function of temperature. Having characterized the stability of the different phases we investigate the energy profile along the transformation path.

MM 18.24 Mon 18:00 P4

**Range Separated Functionals in the Density Functional Based Tight Binding Method** — •Vitalij Lutsker and Thomas A. Niehaus — Universität Regensburg

The density functional based tight binding method (DFTB) is a popular and computationally efficient approximation to the Kohn-Sham density functional theory, showing at the same time useful accuracy. However, being based on the latter, DFTB inherits the problems of DFT due to the approximate nature of the popular local exchange-correlation functionals. Based on the adiabatic connection theorem, hybrid Hartree-Fock-DFT functionals, with mixing ratio dependent on the electron-electron interaction range solve many of the known problems. We intent to implement this approach in the DFTB method.

MM 18.25 Mon 18:00 P4

**Large scale Born-Oppenheimer MD with full local orbital optimization** — •Simon Dubois[1,2] and Mike Payne[2] — [1]Institute of Condensed Matter and Nanosciences, UCL, Louvain-La-Neuve, Belgium — [2]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

To predict sensible trajectories and ensemble averages within the Born-Oppenheimer approximation requires to solve the self-consistent Kohn-Sham equations at each MD steps. To determine the ground- state electronic structure hence dominates the computational effort. The number of cycles required to reach self-consistency can be substantially reduced by using a good initial guess for the electronic degrees of freedom (EDF). Here we investigate various schemes that enable an efficient use of the MD history in order to speed-up BOMD calculations with full local orbital optimization. Extrapolation algorithms are compared with time-reversible propagators of EDF and tensorial corrections applied to density kernels. Multiple time- steps integrators associated with variable levels of local orbitals optimization are also considered.

MM 18.26 Mon 18:00 P4

**C, N and H binding energies in Fe2Nb Laves** — •Alvin Noe Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Germany

The family of Laves phases are interesting from a technological point of view because of their capability for hydrogen storage and their strengthening effect in steel. Although their bulk properties are well understood, the solubility of light elements in these compounds is still unclear. This is due in part to their complex defect structure and the limitations of current experimental techniques for light elements. In this study, we use density functional theory (DFT) to calculate the solubility of C, N and H at the different interstitial sites in the $Fe_2Nb$ C14 Laves phase. Our results suggest that the light elements prefer the voids centered at the triangles shared by two adjacent tetrahedral elements over the centers of these tetrahedra due to the slightly larger volume. Moreover, the binding energies are also dependent on the number of Nb nearest neighbors which is consistent with the high affinity of C, N and H to Nb. Our results suggest a considerable solubility of N and H in $Fe_2Nb$. For C, we observe a weaker solubility which we attribute to the increased strain that is apparent as increased bond lengths.

MM 18.27 Mon 18:00 P4

**Electromagnetic field distribution in composite materials: Are there hot spots?** — •Cintia Hartmann[1], Béatrice Hallouet[1], Romanus Dyczij-Edlinger[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2 Experimentalphysik Universität des Saarlandes Campus E2 6 D-66123 Saarbrücken — [2]Lehrstuhl für Theoretische Elektrotechnik Universität des Saarlandes Campus C6 3 D-66123 Saarbrücken

We numerically investigate electromagnetic field distributions in composite materials. For that purpose, we use a commercial software (CST MICROWAVE STUDIO) to simulate a rectangular waveguide filled with an inhomogeneous medium. This medium consists of a lossy dielectric material, with a volume concentration of about 10%, dispersed in a non-lossy matrix. We simulate different microstructures, from statistical to non statistical (agglomerates) spatial distributions of particles. The simulation gives us simultaneously access to the electromagnetic field and to the effective permittivity ($\varepsilon_{eff}$ through the S-Parameter). We check the local variation of the electric field and of energy disipation in order to find out, whether so-called hot spots exist.

MM 18.28 Mon 18:00 P4

**Bestimmung der Nachweisgrenze bei der Tiefenprofilierung von Fluor in TiAl mittels PIGE** — •Daniel Brenner[1], Hans-Eberhard Zschau[2], Sven Neve[1] und Lothar Schmidt[1] — [1]Institut für Kernphysik, Frankfurt a.M., Deutschland — [2]Dechema-Forschungsinstitut, Frankfurt a.M., Deutschland

Die Modifizierung der Oberflächen von Titan-Aluminium-Legierungen mit Fluor verbessert die Oxidationsbeständigkeit bei hohen Temperaturen. Bei einem neuen Verfahren des Recyclings des Werkstoffs werden geringe Mengen $CaF_2$ zugesetzt. Auch dies könnte zu einem erfolgreichen Oxidationsschutz führen.

Um einen erfolgreichen Halogeneffekt für geringe Konzentrationen von Fluor nachweisen oder widerlegen zu können, muss Fluor bei Konzentrationen im ppm-Bereich zerstörungsfrei nachgewiesen werden können. Dazu wurden $TiAl$-Proben mit geringen Mengen Fluor oberflächennah implantiert. Durch Mehrfachimplantationen kann ein Bereich annähernd konstanter Fluor-Konzentration realisiert werden. Die Technik der Proton Induced Gamma Emission (PIGE) diente zum Nachweis der implantierten Profile. Die Nachweisgrenze unter den Bedingungen der zerstörungsfreien Tiefenprofilierung des bisher üblichen Messsystems mit $NaI$-Detektor und VKA wurde auf 400 ppm bestimmt und nach Umstieg auf digitale Datenaufnahme weiter verbessert. Es wurden sowohl mit Fluor implantierte $TiAl$-Proben, als auch Proben aus recyceltem $TiAl$ untersucht.

MM 18.29 Mon 18:00 P4

**Instabilities during frictional sliding** — •Marc Weikamp[1], Robert Spatschek[1], Efim Brener[2,3], Eran Bouchbinder[3], and Yohai Bar Sinai[3] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100, Israel

The quantitative description of frictional processes ranging from laboratory experiments up to geological events is most commonly described in the framework of the rate-and-state theory of friction. This theory goes beyond the concept of static and dynamic friction coefficients alone and takes into account both a direct effect – a velocity-dependence of the dynamic friction coefficient – as well as an indirect effect via the ageing of microcontacts between the sliding surfaces. It can predict velocity weakening effects, which lead to stick-slip motion. Moreover, the theory successfully describes many features and a rich variety of effects during real earthquake events. Here we show that the standard rate-and-state theory leads to a new and unexpected high frequency instability on the velocity strengthening branch, which is conventionally considered to be stable. Linear stability analyses are applied to situations of infinitely thick and finite height samples, which are dragged over a rigid substrate. The findings are supplemented by finite element simulations of frictional phenomena to explain the occurrence of "slow earthquakes".

MM 18.30 Mon 18:00 P4

**In-situ TEM fracture tests of nanoscale multilayers** — •Christian Meckenhäuser, Andreas Kelling, Inga Knorr, Tobias Liese, Hans-Ulrich Krebs, and Cynthia A. Volkert — Institute for Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany

Nanocomposite materials are commonly used in many different applications due to their unique combinations of material properties. Here, we try to understand the mechanism of fracture in nanocomposites and the influences of interfaces on fracture in order to learn how to separate nanoscale materials efficiently. By varying the layer thicknesses a possible length scale depend behavior of fracture in nanoscale multilayer systems can be tested. The multilayers consist of nanocrystalline Ti and amorphous $ZrO_2$, both deposited by pulsed laser deposition. The mechanical properties of the multilayer samples have been determined using Berkovich indentation and microcompression tests. The interfaces of the multilayer system are very sharp and smooth and the layer thicknesses of each material can by varied between 10 and 100 nm resulting in a perfect set of different samples for the fracture tests. We deform these multilayers with a specially designed in-situ setup inside a TEM using an STM holder which allows for stable and controllable crack growth. Initial studies on samples with 100 nm thick layers show that the cracks form at a notch created with the FIB and run through the middle of a Ti layer. The crack may jump to a neighboring Ti layer by forming a shear band in the intervening $ZrO_2$ layer. In this presentation we will show preliminary results of fracture tests.

MM 18.31 Mon 18:00 P4

**Structure and thermal stability of HPT-processed Cu-16 at.%Al** — •Nazar Ibrahim, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-University Münster,Wilhelm-Klemm-Str. 10, 48149 Münster

Severe plastic deformation is an effective tool for production ultrafine grained materials with extraordinary mechanical properties, corresponding to a high strength and relatively good ductility. In this work, structure modification by high pressure torsion (HPT) and the thermal stability of the resulting microstructure are investigated for the Cu16 at.% Al alloy. For this alloy, a propensity for five-fold twinning has recently been reported [X.H. An, et al., Scripta Materialia 64 (2011) 249]. Disks with a thickness of 0.8 mm and diameter of 10 mm were processed via HPT for 2, 5, 10 and 20 revolutions at room temperature under hydrostatic pressure levels of 2, 4 and 6 GPa and a rotational speed of 1 rpm. Structural and thermal analyses 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. Due to the low stacking fault energy in Cu84Al16, twinning makes a significant contribution to plasticity during HPT. The results are discussed with respect to the reported five-fold twinning in this alloy.

MM 18.32 Mon 18:00 P4

**Microstructural analysis of the creep behavior of directionally solidified eutectic NiAl-Cr** — •Antje Krüger, Michael Klimenkov, and Anton Möslang — Institute for Applied Materials - Applied Materials Physics, Karlsruhe Institute of Technology (KIT)

NiAl with its low creep resistance at T > 600 °C can be strengthened by the refractory element Chromium. The directionally solidified eutectic composite NiAl-34Cr (at%) forms long Cr-fibers with diameters between 200 nm and 700 nm depending on the production process. NiAl-Cr shows at high temperatures a better oxidation and creep resistance and a reduced brittle to ductile transition temperature (BDTT) than the binary system NiAl. Typical applications for this material would comprise devices in gasturbines and aeroplane turbines to get an improved energy efficiency.

In our study we present first results of creep tests measured at constant compressive loads and constant temperatures above 700 °C under vacuum conditions. The cylindrical specimens were manufactured by wire electro-discharge machining with a diameter of 3mm and a length of 6 mm. The microstructure of the tested specimens is analyzed by TEM. With this facility we can have a look on the microstructure to find out which mechanisms are responsible for the deformation and how the Cr-fibers strengthen the NiAl-matrix. Further investigations are done by EDX measurements and selected area diffraction patterns (SADP) to get information on the chemical composition and the crystal orientation of the NiAl matrix, the Cr fibers and the interface.

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MM 18.33 Mon 18:00 P4

**PAC studies of uniaxial compressive stressed zinc, titanium, rutile, $Ti_2AlN$, and $Nb_2AlC$** — •Christoph Brüsewitz[1], Daniel Jürgens[1], Ulrich Vetter[1], Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

Polycrystalline zinc, titanium, rutile, and the MAX phases $Ti_2AlN$ and $Nb_2AlC$ were studied with the perturbed angular correlation (PAC) method using $^{111}In/^{111}Cd$ as probe atom. The electric field gradient (EFG) at room temperature was studied as function of mechanical deformation caused by a uniaxial compressive load. A reversible and an irreversible increase in the distribution width of the EFG, visible as a damping of the PAC spectrum, were found under load and after releasing the load, respectively. Annihilation of dislocations, in agreement with the proposed incipient kink band (IKB) mechanism, as well as elastic deformation are considered to contribute to the reversible behavior. The irreversible behavior is caused by a permanent increase in dislocation and point defect density. The deformation induced broadening of the EFG can be recovered by post-annealing of the deformed

sample.

MM 18.34 Mon 18:00 P4

**In-situ TEM deformation of $Ti_3SiC_2$- MAX phase** — •Mona-Christin Maass, Burkhard Roos, and Cynthia A. Volkert — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany

MAX phases are layered alloys consisting of a transition metal, an A-group element, and carbon (or nitrogen). They are interesting candidates for technical application because of their combined properties: electrically and thermally conductive like metals, but also stiff, heat-resistant, and brittle like ceramics.

In-situ TEM experiments are performed to examine the plastic deformation of $Ti_3SiC_2$, where dislocation motion is strongly constrained in the basal planes, and to gain insights into the 2-dimensional dynamics of dislocations. For these experiments samples were prepared by conventional thinning with dimpling and Ar ion milling, and also by FIB milling. The samples contained an initial high density of dislocations and were deformed in-situ by loading them with a piezo actuated tungsten tip. These in-situ experiments showed that dislocations move under loading and are able to leave the sample at its free surfaces. Based on crystallographic investigations and TEM post-mortem analysis the slip planes and slip directions of the dislocations and their interactions with existing defects in $Ti_3SiC_2$ is discussed. Although these observations are specific to $Ti_3SiC_2$, other MAX phases are likely to behave similarly because they all have similar layered, hexagonal structures.

MM 18.35 Mon 18:00 P4

**Using molecular dynamics modeling to determine the free energy of melts and intermetallic compounds of binary alloys** — •Mohammed Guerdane — Karlsruhe Institute of Technology (KIT) Institute of Applied Materials - Reliability of Components and Systems (IAM-ZBS)

Knowledge of the dependence of the free energy (FE) on temperature and density is a necessary pre-requisite to understand the thermodynamics of phase transformations -like solidification- of binary or multicomponent melts. We present here an atomistic approach aimed at determining the free energy of binary alloy liquids $f_{liq}$ by combining the quasiharmonic approximation, applied for solids, with the liquid-solid coexistence method. Despite of its simplicity, this approach is able to deliver an accurate phase diagram and to describe with high reliability phase transformations. This is demonstrated by linking molecular dynamics simulations to phase-field modeling (based on $f_{liq}$) in a quantitative study of solidification and melting kinetics. This approach would be a valuable alternative to the mostly sophisticated and costly free energy methods.

MM 18.36 Mon 18:00 P4

**Waiting time statistics indicating crossover from 3D uncorrelated nano shear bands to cooperative shear motion** — Jon-Olaf Krisponeit, •Sebastian Pitikaris, Karina E. Avila, Stefan Küchemann, Antje Krüger und Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We investigated the post-elastic creep deformation of $Pd_{77.5}Cu_6Si_{16.5}$ metallic glas ribbons via Dynamical Mechanical Analysis, i.e. we recorded its strain response over time after exerting a uniaxial stress jump. Macroscopically, one observes a smooth strain curve comprising of elastic, anelastic and plastic contributions. On a finer scale, however, the creep curve is made up of steplike jumps rather than proceeding continuously. We approach the statistical properties of the underlying slip events using a novel waiting time analysis. These show a power law distribution similar to those observed for other systems exhibiting avalanche dynamics e.g. Barkhausen noise or fracture in crystals. In long-time experiments we observed a crossover between two distinct power law regimes. We ascribe the first regime to the stress-assisted formation of 3D independent avalanches of shear transformation zones, the fundamental microscopic unit of deformation. The transition to a second power-law regime indicates the onset of cooperative 2D nano shear band motion. We acknowledge financial support for this work by DFG via SFB 602 and FOR 1394 and the German-Israeli Foundation.

MM 18.37 Mon 18:00 P4

**Electronic properties of metallic gallium up to 4 GPa as studied with new anvil-cell NMR** — •Thomas Meier and Jürgen Haase — Universität Leipzig, Institut für Experimentelle Physik II

A new approach to nuclear magnetic resonance under pressures of several GPa is developed and is used to investigate the response of the electronic states, as well as the atomic motion in gallium (Ga) metal. Liquid Ga (below 2 Gpa) was studied, as well as solid Ga in the cubic Ga-II phase at pressures up to 4 GPa. We found distinct deviations from what is expected for a free electron liquid, which cannot be explained with current theories. The change in the electronic properties upon the pressure inducing solidification at 2 GPa, indicates a dramatic change in the electronic density of states at the Fermi level, which is a characteristic feature of anomalous melting metals. The investigation of the nuclear spin-lattice relaxation allows us also to determine the correlation time of the fluctuations of the electric field gradient at the nuclei produced by the high atomic mobility in the melt. We find the correlation time to increase linearly with pressure, up to the phase transition. Additionally, the observed freezing and melting behaviour of liquid gallium/gallium I at various pressures displayed a distinct hysteresis, indicating pressure induced alterations in the crystallisation behaviour of volume constricted gallium metal.

MM 18.38 Mon 18:00 P4

**Hardness measurements of shear bands in the bulk metallic glass $Pd_{40}Ni_{40}P_{20}$ by Nanoindentation** — •Niklas Nollmann, Jörn Leuthold, and Gerhard Wilde — WWU Münster, Deutschland

In metallic glasses the hardness is influenced by the deformation state of the glass. For example in a sample deformed by rolling, the hardness is lower than in an undeformed sample. During the process of deformation the stress is localized in shear bands that are expected to have lower elastic modulus and lower hardness. In order to experimentally assess this hypothesis, nanoindentation was utilized. There for we prepared cold rolled metallic glass samples to obtain a defined state. Shear bands are produced, which are easy visible on the polished surface of the Sample. The hardness has been measured by two different ways. Firstly we made a number of defined nanoindents directly on top of the shear bands without polishing the sample. Secondly the sample has been polished before the nanoindentation measurements. SEM micrographs were taken before the polishing and finally after the nanoindentation process. By image correlation of these SEM micrographs, the position of the shear bands could be determined. The hardness of every indent was calculated in order to estimate the hardness of the shear bands.

MM 18.39 Mon 18:00 P4

**Effect of shear localization on atomic transport and mechanical damping in a Pd40Ni40P20 bulk metallic glass** — •Isabelle Binkowski[1], Igor S. Golovin[2], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]1- Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]2- Technological University 'MISiS', Leninsky ave.4, 119049 Moscow, Russia

Bulk metallic glasses feature beneficial properties which are promising for applications, because of which they have received increasing attention. Metallic glasses exhibit mechanical properties such as high strength and hardness, however, this advantage is impeded by the fact that their plasticity appears to be extremely limited. The plastic deformation is localized in thin regions, called shear bands, with widths from 10nm to 50 nm, whose extension lead to catastrophic failure. Despite their obvious importance, there exist several open issues concering the initiation, propagation, kinetics and general comprehension of shear banding. In the present study, the characteristics of shear bands in a Pd40Ni40P20 bulk metallic glass are investigated more precisely utilizing the radiotracer technique to measure atomic transport in shear bands. Additionally, combining these experimental results with calorimetric measurements and a mechanical spectroscopy study gives insight into the time-dependence and the impact of structural changes on diffusion and damping capability of the metallic glass.

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