

Metal and Material Physics Division Fachverband Metall- und Materialphysik (MM)

Jörg Neugebauer
Max-Planck-Institut für
Eisenforschung, GmbH
Max-Planck-Straße 1
40237 Düsseldorf
neugebauer@mpie.de

Overview of Invited Talks and Sessions

(Lecture rooms H38, H39, H51, H52, and H53; Poster B3)

Invited Talks

MM 16.1	Tue	9:30–10:00	H38	Critical stresses in intermittent plasticity and the transition to macroscopic yield — •PETER DERLET, ROBERT MAASS
MM 27.1	Wed	9:30–10:00	H38	The secret of shear bands — •HARALD RÖSNER
MM 38.1	Wed	15:00–15:30	H38	Models for adhesion, friction and wear across the scales — •LARS PASTEWKA, PETER GUMBSCH, MICHAEL MOSELER, GIANPIETRO MORAS, ANKE PEGUIRON, MARK ROBBINS
MM 44.1	Wed	18:30–19:00	H38	Design of ductile Mg alloys based on combined high resolution electron microscopy experiments and ab initio calculations — •STEFANIE SANDLÖBES, MARTIN FRIÁK, ZONGRUI PEI, TALAL AL-SAMMAN, SANDRA KORTEKERZEL, JÖRG NEUGEBAUER, DIERK RAABE
MM 45.1	Wed	19:00–19:30	H38	Computer simulation of bulk-metallic glasses under shear: From inhomogeneous flow patterns to mechanical properties — •JUERGEN HORBACH, GAURAV PRAKASH SHRIVASTAV, PINAKI CHAUDHURI
MM 47.1	Thu	9:30–10:00	H38	Nondestructive micro/nanostructure analysis using diffraction — •MATTEO LEONI
MM 57.1	Thu	15:00–15:30	H38	Virtual diffraction as a tool to investigate nanostructured materials — •JÜRGEN MARKMANN

Invited talks of the joint symposium SYCE

See SYCE for the full program of the symposium.

SYCE 1.1	Mon	15:00–15:30	H1	Multicaloric effects in metamagnetic Heusler materials — •ANTONI PLANES
SYCE 1.2	Mon	15:30–16:00	H1	Multicaloric effect in biological systems: a case of nerve action — •MATJAZ VALANT, LAWRENCE J. DUNNE, ANNA-KARIN AXELSSON, FLORIAN LE GOUPIL, GEORGE MANOS
SYCE 1.3	Mon	16:00–16:30	H1	Optimizing the electrocaloric effect by first-principles simulations: The role of strain and defects — •ANNA GRÜNEBOHM
SYCE 1.4	Mon	16:45–17:15	H1	Giant inverse barocaloric effects in ferroelectric ammonium sulphate — POL LLOVERAS, ENRIC STERN-TAULATS, MARIA BARRIO, JOSEP LLUIS TAMARIT, SAM CROSSLEY, WEI LI, VLADIMIR POMJAKUSHIN, ANTONI PLANES, LLUIS MAÑOSA, NEIL MATHUR, •XAVIER MOYA
SYCE 1.5	Mon	17:15–17:45	H1	TiNiCu-based thin films for elastocaloric cooling — •ECKHARD QUANDT, CHRISTOPH CHLUBA

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — •ALLAN H MACDONALD
----------	-----	------------	----	--

SYES 1.2	Fri	10:00–10:30	H1	Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — ●JAIRO SINOVA
SYES 1.3	Fri	10:30–11:00	H1	Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — ●EWELINA HANKIEWICZ
SYES 1.4	Fri	11:15–11:45	H1	Engineering Topological Quantum States: From 1D to 2D. — ●JELENA KLINOVAJA
SYES 1.5	Fri	11:45–12:15	H1	Skyrmions – Topological magnetization solitons for future spintronics — ●STEFAN BLÜGEL

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H38	Invited talk Olson
MM 2.1–2.4	Mon	10:15–11:45	H38	Topical session: Integrated computational materials engineering for design of new materials I
MM 3.1–3.5	Mon	10:15–11:45	H39	Interfaces I: Mechanical properties
MM 4.1–4.4	Mon	10:15–11:30	H52	Liquid and Amorphous Metals I: Glassy dynamics
MM 5.1–5.4	Mon	10:15–11:30	H53	Nanomaterials I: Mechanics
MM 6.1–6.6	Mon	11:30–13:00	H52	Liquid and Amorphous Metals II: Shear bands
MM 7.1–7.5	Mon	11:30–12:45	H53	Transport I: Electronic and thermal transport
MM 8.1–8.5	Mon	11:45–13:15	H38	Topical session: Integrated computational materials engineering for design of new materials II
MM 9.1–9.4	Mon	11:45–12:45	H39	Interfaces II: Segregation and embrittlement
MM 10.1–10.5	Mon	15:00–17:45	H1	SYCE: Caloric effects in ferroic materials
MM 11.1–11.7	Mon	15:45–18:00	H39	Topical session: Integrated computational materials engineering for design of new materials III
MM 12.1–12.7	Mon	15:45–17:45	H51	Frontiers of Electronic Structure Theory: Focus on Topology and Transport
MM 13.1–13.6	Mon	15:45–17:30	H52	Liquid and Amorphous Metals III: Mechanical properties
MM 14.1–14.6	Mon	15:45–17:30	H53	Transport II: Atomic and ionic transport
MM 15.1–15.39	Mon	18:00–20:00	Poster B3	Poster session I
MM 16.1–16.1	Tue	9:30–10:00	H38	Invited talk Derlet
MM 17.1–17.3	Tue	10:15–11:45	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science I
MM 18.1–18.4	Tue	10:15–11:45	H39	Topical session: Integrated computational materials engineering for design of new materials IV
MM 19.1–19.5	Tue	10:15–11:45	H52	Mechanical Properties I
MM 20.1–20.4	Tue	10:15–11:45	H53	Topical session: Caloric Effects in ferroic materials I - Magnetocalorics
MM 21.1–21.6	Tue	11:45–13:15	H38	Microstructure and Phase Transformations I
MM 22.1–22.7	Tue	11:45–13:30	H39	Topical session: Integrated computational materials engineering for design of new materials V
MM 23.1–23.6	Tue	11:45–13:15	H52	Mechanical Properties II
MM 24.1–24.5	Tue	11:45–13:15	H53	Topical session: Caloric Effects in ferroic materials II - Methods and Applications
MM 25.1–25.7	Tue	14:00–16:00	H24	Frontiers of Electronic Structure Theory: Focus on Topology and Transport I
MM 26.1–26.43	Tue	18:30–20:30	Poster B3	Poster session II
MM 27.1–27.1	Wed	9:30–10:00	H38	Invited talk Rösner
MM 28.1–28.4	Wed	10:15–11:45	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science II - Atomic structure and defects I
MM 29.1–29.5	Wed	10:15–11:45	H39	Topical session: Caloric effects in ferroic materials III - Electrocalorics
MM 30.1–30.4	Wed	10:15–11:30	H52	Structural Materials I
MM 31.1–31.5	Wed	10:15–11:45	H53	Functional materials I: Supercapacitors and batteries I
MM 32.1–32.10	Wed	10:30–13:00	H24	Frontiers of Electronic Structure Theory: Focus on Topology and Transport II
MM 33.1–33.4	Wed	11:45–13:15	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science III - Atomic structure and defects II

MM 34.1–34.3	Wed	11:45–12:45	H39	Topical session: Caloric effects in ferroic materials IV - Heuslers
MM 35.1–35.4	Wed	11:45–12:45	H52	Structural Materials II
MM 36.1–36.5	Wed	11:45–13:00	H53	Functional materials II: Batteries II
MM 37.1–37.12	Wed	15:00–18:30	H24	Frontiers of Electronic Structure Theory: Focus on Topology and Transport III
MM 38.1–38.1	Wed	15:00–15:30	H38	Invited talk Pastewka
MM 39.1–39.11	Wed	15:00–18:15	H40	Biomaterials and Biopolymers I (joint session CPP/BP/MM)
MM 40.1–40.6	Wed	15:45–18:00	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science IV - Atomic structure and defects III
MM 41.1–41.8	Wed	15:45–18:00	H52	Methods in Computational Materials Modelling I: Ab initio thermodynamics
MM 42.1–42.6	Wed	15:45–17:30	H53	Functional materials III: Actuators, sensors and functional devices
MM 43.1–43.7	Wed	18:15–20:30	Poster A	Frontiers of Electronic-Structure Theory: Focus on Topology and Transport
MM 44.1–44.1	Wed	18:30–19:00	H38	Invited talk Sandloebes
MM 45.1–45.1	Wed	19:00–19:30	H38	Invited talk Horbach
MM 46	Wed	19:45–20:45	H38	Annual General Assembly of the MM Division
MM 47.1–47.1	Thu	9:30–10:00	H38	Invited talk Leoni
MM 48.1–48.4	Thu	10:15–11:45	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science V - Biological and Electronic Materials
MM 49.1–49.5	Thu	10:15–11:30	H39	Nanomaterials II: Synthesis
MM 50.1–50.5	Thu	10:15–11:45	H53	Methods in Computational Materials Modelling II: Microstructure evolution
MM 51.1–51.9	Thu	10:30–13:15	H24	Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV
MM 52.1–52.5	Thu	11:45–13:15	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science VI - Structural transitions
MM 53.1–53.5	Thu	11:45–13:00	H39	Microstructure and Phase Transformations II
MM 54.1–54.5	Thu	11:45–13:00	H52	Biomaterials and Biopolymers II (Joint CPP/BP/MM)
MM 55.1–55.5	Thu	11:45–13:00	H53	Methods in Computational Materials Modelling III: Machine learning and statistics
MM 56.1–56.13	Thu	15:00–18:15	H24	Frontiers of Electronic Structure Theory: Focus on Topology and Transport V
MM 57.1–57.1	Thu	15:00–15:30	H38	Invited talk Markmann
MM 58.1–58.5	Thu	15:00–16:15	H45	Biomaterials and Biopolymers III (Joint Session with CPP/BP/MM)
MM 59.1–59.8	Thu	15:45–18:30	H38	Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science VII - Nanomaterials
MM 60.1–60.5	Thu	15:45–17:00	H39	Microstructure and Phase Transformations III
MM 61.1–61.4	Thu	15:45–16:45	H52	Functional materials IV: Batteries III
MM 62.1–62.7	Thu	15:45–17:45	H53	Methods in Computational Materials Modelling IV: Method development
MM 63.1–63.5	Fri	9:30–12:15	H1	Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:45-20:45 H38

MM 1: Invited talk Olson

Time: Monday 9:30–10:00

Location: H38

Topical Talk

MM 1.1 Mon 9:30 H38

Computational Materials Design: From Genome to Flight —

•GREG OLSON — Northwestern University, Evanston, IL, USA

The numerical implementation of established materials science principles in the form of purposeful engineering tools has brought a new level of integration of the science and engineering of materials. Building on a system of fundamental databases now known as the Materials Genome, parametric materials design has integrated materials science, applied mechanics and quantum physics within a systems engineering framework to create a first generation of designer "cyberalloys" that have

now entered successful commercial applications, while the DARPA-AIM initiative has broadened computational materials engineering to address acceleration of the full materials development and qualification cycle. Integration with the full suite of fundamental databases and models has demonstrated the historic milestone of greatly accelerated flight qualification for two aircraft landing gear steels. In support of the US Materials Genome Initiative, the new NIST-sponsored CHiMaD Center for Hierarchical Materials Design expands the scope of genomic materials design across materials classes. Under the DARPA Open Manufacturing program, the scope of AIM qualification is being extended to additively manufactured components.

MM 2: Topical session: Integrated computational materials engineering for design of new materials I

Time: Monday 10:15–11:45

Location: H38

Topical Talk

MM 2.1 Mon 10:15 H38

High-Throughput Computational Search for Precipitation Hardened Alloy Systems —

•CHRIS WOLVERTON — Dept. of Materials Science and Eng., Northwestern University, Evanston, IL USA 60208

The search for high-strength alloys and precipitation hardened systems has largely been accomplished through Edisonian trial and error experimentation. Here, we present a novel strategy using high-throughput computational approaches to search for promising precipitate/alloy systems. We perform density functional theory (DFT) calculations of an extremely large space of ~200,000 potential compounds in search of effective strengthening precipitates for a variety of different alloy matrices, e.g., Fe, Al, Mg, Ni, Co, and Ti. Our search strategy involves screening phases that are likely to produce coherent precipitates (based on small lattice mismatch) and are composed of relatively common alloying elements. When combined with the Open Quantum Materials Database (OQMD, oqmd.org), we can computationally screen for precipitates that either have a stable two-phase equilibrium with the host matrix, or are likely to precipitate as metastable phases. Our search results produce (for the structure types considered) nearly all currently known high-strength precipitates in a variety of fcc, bcc, and hcp matrices, thus giving us confidence in the strategy. In addition, we predict a number of new, currently-unknown precipitate systems that should be explored experimentally as promising high-strength alloy chemistries.

Heat capacity of the quaternary Q phase in Al-Cu-Mg-Si: a combined ab-initio, phonon and compound energy formalism approach —•ALI ZENDEGANI¹, FRITZ KÖRMANN¹, TILMANN HICKEL¹, BENGT HALLSTEDT², and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Rheinisch-Westfälische Technische Hochschule Aachen, Aachen, Germany

The Q phase is an important quaternary precipitate in aluminum-based alloys that contain Mg, Si and Cu. These alloys belong to the most promising materials in automotive and aircraft engineering. To tailor their mechanical characteristics via heat treatments, a precise knowledge of their precipitation properties is essential.

In order to achieve an improved thermochemical parameter set of the Q phase, we have performed a combined first-principles, phonon and compound energy formalism approach on this phase to investigate its heat capacity. For a fair comparison with available experimental data, the impact of lattice vibrations on the site occupancy of sublattices has also been taken into account. Excellent agreement with experimental data demonstrates the high predictive power of our first-principles approach [1].

[1] A. Löffler, A. Zendegani, J. Gröbner, M. Hampl, R. Schmid-Fetzer, H. Engelhardt, M. Rettenmayr, F. Körmann, T. Hickel, J. Neugebauer, Journal of Phase Equilibria and Diffusion, in press

MM 2.2 Mon 10:45 H38

Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration —ANDREAS HERZ¹, •MARTIN FRIÁK^{2,3}, DIANA ROSSBERG¹, MARTINA HENTSCHEL¹, FELIX THESKA¹, DONG WANG¹, DAVID HOLEC⁴, MOJMÍR ŠOB^{3,2,5}, OLDŘICH SCHNEEWEISS², and PETER SCHAAP¹ — ¹TU Ilmenau, Ilmenau, Germany — ²Institute of Physics of Materials, AS CR, Brno, Czech Republic — ³CEITEC MU, Masaryk University, Brno, Czech Republic — ⁴Montanuniversität Leoben, Leoben, Austria — ⁵Dept. of Chem., Faculty of Science, Masaryk University, Brno, Czech Republic

Solid-state dewetting is used to fabricate supersaturated, submicron-sized Au-Ni solid solution particles out of thin Au/Ni bilayers by means of a rapid thermal annealing technique. Phase separation in such particles is studied with respect to their equilibrium crystal (or Wulff) shape by subsequent annealing at elevated temperature. It is found that {100} faceting planes of the equilibrated particles are enriched with Ni and {111} faces with Au. Both phases are treated by quantum-mechanical calculations in combination with an error-reduction scheme that was developed to compensate for a missing exchange-correlation potential that would reliably describe both Au and Ni. The observed phase configuration is then related to the minimization of strongly anisotropic elastic energies of Au- and Ni-rich phases and results in a rather unique nanoparticle composite state that is characterized by nearly uniform value of elastic response to epitaxial strains all over the faceted surface. This work demonstrates a route for studying features of physical metallurgy at the mesoscale (APL 107 (2015) 073109).

MM 2.3 Mon 11:00 H38

MM 2.4 Mon 11:15 H38

Numerical multi-criteria optimization methods for alloy design: Development of new high strength nickel-based superalloys and experimental validation —

•RALF RETTIG, ALEXANDER MÜLLER, NILS C. RITTER, and ROBERT F. SINGER — Institute of Science and Technology of Metals, Department of Materials Science and Engineering, University of Erlangen, Martensstr. 5, D-91058 Erlangen, Germany

A new approach for the design of optimum balanced metallic alloys is presented. It is based on a mathematical multi-criteria optimization method which uses different property models to predict the alloy behavior in dependency of composition. These property models are mostly based on computational thermodynamics (CALPHAD-method). The full composition range of the alloying elements can be considered using these models. In alloy design usually several contradicting goals have to be fulfilled. This is handled by the calculation of so-called Pareto-fronts. The aim of our approach is to guide the experimental research towards new alloy compositions that have a high probability of having very good properties. Consequently the number of required test alloys can be massively reduced. The approach will be demonstrated for the computer-aided design of a new Re-free superalloy with nearly identical creep strength as that of Re-containing superalloys. Our starting point for the design was to maintain the good properties of the gamma prime-phase in well-known alloys like CMSX-4 and to maximize the solid solution strengthening of W and Mo. The presented experimental measurements proof the excellent properties.

15 min. coffee break

MM 3: Interfaces I: Mechanical properties

Time: Monday 10:15–11:45

Location: H39

MM 3.1 Mon 10:15 H39

Migration mechanisms of grain boundaries deviating from the symmetric tilt orientation — ●SHERRI HADIAN¹, BLAZEJ GRABOWSKI¹, CHRIS RACE², and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — ²Dalton Nuclear Institute, University of Manchester, Manchester M13 9PL, United Kingdom

We have studied the migration kinetics and atomistic mechanisms of mixed tilt and twist grain boundaries systematically deviated from the symmetric tilt $\Sigma 7 \langle 111 \rangle \{1\ 2\ 3\}$ orientation as they constitute the majority of experimentally observed mobile grain boundaries. Using physically converged simulations and investigating dense motion snapshots in 3D, we find unique characteristic mechanisms in the motion of non-symmetric grain boundaries as compared with the symmetric one. The mixed grain boundaries show nano-faceting, which enables two heterogeneous atomistic migration mechanisms and critically changes the previously reported island nucleation mechanism in the symmetric $\Sigma 7$ tilt boundary [1]: Depending on the orientation of the nano-facets/steps either a double kink nucleation and propagation or a pure kink flow drives the motion. We show that these atomistic mechanisms are the origin of the observed change from a strongly non-Arrhenius behavior towards a more Arrhenius one and subsequently a change in the asymptotic behavior of the migration barrier at low driving forces as we change the grain boundary from a symmetric tilt to a general mixed one. In the end, connections were made between grain boundary migration processes and those of the surface epitaxial growth.

MM 3.2 Mon 10:30 H39

Shear Modulus of grain boundaries in relaxed and deformation-modified states — ●LISA NEIER¹, SERGIY DIVINSKI¹, ANANTHA PADMANABHAN², and GERHARD WILDE¹ — ¹Institut für Materialphysik, Westfälische-Wilhelms-Universität, 48149 Münster — ²University of Hyderabad, India

A comparison of properties in materials subjected to severe plastic deformation or steady state superplastic flow shows several similarities especially with respect to the interface response to the deformation, such as grain boundary sliding events. Making use of this idea, we propose to describe the experimentally observed "high-energy" state of general high-angle grain boundaries in severely plastically deformed materials in terms of a concept of shear localization and extra free volume in the interfaces, with oblates spheroids chosen as basic sliding units.

By performing atomistic simulations of these grain boundaries their response to deformation is analysed. With special focus on shear deformation parallel to the grain boundary plane, properties, such as the local shear modulus of these grain boundaries, are calculated and compared to the properties of relaxed high angle grain boundaries.

MM 3.3 Mon 10:45 H39

Atomistic simulations of planar defects in solids: evaluations of present and new methods for computation of strength of grain boundaries — ●PETR ŠESTÁK^{1,2}, PETR ŘEHÁK^{1,2}, MIROSLAV ČERNÝ^{1,2}, MONIKA VŠIANSKÁ^{1,2}, JIANYING HE³, JAROSLAV POKLUDA², ZHILIANG ZHANG³, and MOJMÍR ŠOB^{1,2,4} — ¹Institute of Physics of Mater., Academy of Sci. of CZ, Brno, CZ — ²CEITEC, Brno, CZ — ³Faculty of Engineering Science and Technology, NTNU, Trondheim, NO — ⁴Faculty of Science, Masaryk University, Brno, CZ

Planar defects like grain boundaries predetermine mechanical properties of polycrystalline materials and, in particular, their strength. Therefore, a lot of effort has been devoted to study these phenomena not only at macroscopic level but also at nano- and atomistic scales using simulations based on DFT. However, such simulations always omitted the Poisson contraction, which leads to relaxation of transverse stresses. In the present study, we propose and test two models

of the tensile tests (including the transverse contraction) on crystals containing planar defects. One model comprises full optimization of the lattice via relaxation of the lateral stress tensor components while the other uses a new, simplified approach. The models are tested and verified for a tensile loading of the $\Sigma 5$ (210) tilt grain boundary in Ni. The comparison of both methods reveals that the results are almost identical. However, our new model allows us to decrease the computational time significantly. Both models are also compared with former approaches where the Poisson contraction was neglected.

MM 3.4 Mon 11:00 H39

Material transfer and its suppression at Al-TiN and Cu-C interfaces from first principles — ●GREGOR FELDBAUER^{1,2,3}, MICHAEL WOLLOCH², PEDRO O. BEDOLLA³, ANDRÁS VERNES^{2,3}, JOSEF REDINGER², and PETER MOHN² — ¹Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ²Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — ³AC2T research GmbH, Wiener Neustadt, Austria

Contacts of surfaces at the atomic length scale are of fundamental interest for a better understanding of nanotribological processes, which are crucial in modern applications from nanoindentation or AFM/FFM to nanotechnologies applied in NEMS/MEMS.

A series of density functional theory (DFT) simulations was performed to investigate the approaching, contact and subsequent separation of two atomically flat surfaces consisting of various materials. Here, interfaces between Al and TiN slabs as well as Cu and C (diamond) slabs were chosen as model systems representing the interaction between soft and hard materials. The approaching and separation were simulated by moving one slab in discrete steps and allowing for relaxations after each step. Various configurations of the surfaces were analyzed at the interfaces. Additionally, the effect of oxygen and hydrogen at the Al and C surface, respectively, was investigated. The performed simulations revealed the influences of these aspects on the adhesion, equilibrium distance, charge distribution and material transfer. Particularly, oxygen and hydrogen showed their potential to suppress material transfer at the examined interfaces.

MM 3.5 Mon 11:15 H39

Influence of patterned stress states on Hydrogen loading in Vanadium thin films studied by electrochemical Hydrogenography — ●ANSHU TYAGI, FLORIAN DÖRING, HANS-ULRICH KREBS, and ASTRID PUNDT — Univ. Göttingen, IMP, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The mechanical stress state of a metal film sensitively affects the chemical potential of Hydrogen in the metal.[1] The stress state can be changed by the adhesion of the metal film to the substrate.[2] Stress sensitive Vanadium thin films act as model systems in this paper.[3] These films are sputter deposited onto transparent glass substrates. Stress modulation is achieved using patterned Palladium and Polycarbonate layers. The Hydrogen uptake in these films is studied using Hydrogenography which monitors the film transparency and reflectivity.[4] These optical properties depend on the Hydrogen concentration via Lambert-Beer's law. We apply this method using electrochemical loading in a light-microscope. This electrochemical Hydrogenography allows to optically probe for the local Hydrogen concentration. Comparative studies on different adhesion conditions are done by in-situ EMF measurements. This provides the related chemical potentials including information about the phase boundaries. The transmission and reflection spectra are discussed with respect to these data. This research is kindly supported by the DFG via SFB1073 and PU131/9-2. [1] S.Wagner, A. Pundt, APL 92 (2008) 051914. [2] A. Pundt et al. Acta Mater. 52 (2004) 1579. [3] E. T. Gutelmacher et al., J Matter Sci. 45 (2010) 6389. [4] R. Gremaud et al., APL 91 (2007) 231916.

15 min. coffee break

MM 4: Liquid and Amorphous Metals I: Glassy dynamics

Time: Monday 10:15–11:30

Location: H52

MM 4.1 Mon 10:15 H52

Experimental evidence for a dynamical crossover in liquid aluminium — ●FRANZ DEMMEL¹ and CHRISTOPH MORKEL² — ¹ISIS Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK — ²Physikdepartment E21, TU Munchen, 85748 Garching, Germany

The temperature dependence of the dynamic structure factor at next-neighbour distances has been investigated for liquid aluminium [1]. This correlation function is a sensitive parameter for changes in the local environment and its Fourier transform was measured in a coherent quasielastic neutron scattering experiment. The zero frequency amplitude decreases in a nonlinear way and indicates a change in dynamics around 1.4 Tmelting. From that amplitude a generalized viscosity can be derived which is a measure of local stress correlations on next-neighbour distances. The derived generalized longitudinal viscosity shows a changing slope at the same temperature range. At this temperature the freezing out of degrees of freedom for structural relaxation upon cooling sets in which can be understood as a precursor towards the solid state. Thermodynamic calculations for the solid state predicted an upper temperature stability limit for the solid phase which corresponds favourable with our observations. That crossover in dynamics of liquid aluminium shows the same signatures as previously observed in liquid rubidium and lead, indicating a universal character. [1] F. Demmel, A. Fraile, D. Szubrin, W.C. Pilgrim and C. Morkel, J.Phys.: Condens. Matter 27 455102 (2015)

MM 4.2 Mon 10:30 H52

Distinct dynamical regimes in a gold-based metallic glass revealed by X-ray photon correlation spectroscopy (XPCS) — ●SIMON HECHLER¹, BEATRICE RUTA², ZACH EVENSON³, MORITZ STOLPE¹, WILLIAM HEMBREE¹, ISABELLA GALLINO¹, and RALF BUSCH¹ — ¹Lehrstuhl für Metallische Werkstoffe, Universität des Saarlandes, Saarbrücken — ²ESRF, Grenoble — ³Heinz Maier-Leibnitz-Zentrum, TU München, Garching

Although structural relaxation is a universal feature of glasses, the atomic-level processes involved still remain a puzzling mystery. XPCS has emerged as a novel technique for studying the microscopic dynamics of non-equilibrium condensed matter, as it enables the investigation of the structural relaxation time by resolving the translational atomic motion in non-equilibrium materials as metallic glasses. Using XPCS experiments, we follow the equilibration from the glass into the supercooled liquid of a gold-based metallic glass. The as-cast alloy shows different dynamical regimes as it approaches the glass transition. At low temperature, the relaxation time appears to be almost temperature independent. Upon heating, closer to the glass transition, the glass shows highly temperature dependent dynamics. In the supercooled liquid region, the material changes the equilibrium dynamics upon cooling to a significantly stronger dynamic behavior, without freezing to a glass. Such crossovers in the dynamics have not been observed in XPCS studies before and suggest the existence of complex structural relaxation mechanisms in this metallic glass forming material.

MM 4.3 Mon 10:45 H52

Atomic-scale structural changes during a liquid-liquid transition in a Zr-based bulk metallic glass forming alloy — ●MORITZ STOLPE¹, SHUAI WEI², ISABELL JONAS³, WILLIAM HEMBREE¹, ZACH EVENSON⁴, FAN YANG³, ANDREAS MEYER³, and RALF BUSCH¹ — ¹Lehrstuhl für Metallische Werkstoffe, Universität des Saarlandes, Saarbrücken — ²Department of Chemistry and Biochemistry, Arizona State University, Tempe — ³Institut für Materialphysik im Weltraum, DLR, Köln — ⁴Heinz Maier-Leibnitz Zentrum, TU München, Garching

Liquid-liquid phase transitions (LLTs) are considered as a possible source to explain anomalous changes in the viscous behavior, a phenomenon known as fragile-strong transition.

Using synchrotron X-ray scattering combined with electrostatic levitation we investigated the structural evolution of Zr-based metallic glass forming alloy from above the liquidus temperature down to the glass transition temperature Tg. Our study reveals a LLT from a less ordered high temperature to a more ordered low temperature phase which, thermodynamically, manifests as a smeared-out peak in the heat capacity. Although no notable density change is observed, marked structural changes in both, short- (SRO) and medium range order (MRO) occur. Our results imply that in particular the structural evolution at MRO is related to the experimentally observed change in the viscous behavior. This is in agreement with the conception that the viscous slowdown is related to an extension of MRO through an aggregation of energetically-preferred atomic clusters.

MM 4.4 Mon 11:00 H52

Thermodynamic Properties of Zr- and Au-based Bulk Metallic Glasses Low Temperatures — ●ANDREAS REIFENBERGER¹, MAHMOUD ABDEL-HAFIEZ², ANDREAS FLEISCHMANN¹, ANDREAS REISER¹, and CHRISTIAN ENSS¹ — ¹Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg — ²Physikalisches Institut, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

The origin of low temperature excitations in bulk metallic glasses is still an open question. We report on measurements of both low-temperature specific heat C_p and thermal conductivity κ of two model glasses based on Au and Zr (Au-BMG and Zr-BMG, respectively) in the temperature range from 1K to room temperature. We find pronounced low temperature anomalies in the phononic specific heat C_{ph} , which are attributed to localized harmonic vibration modes. These Einstein modes act as additional scattering centers as can be seen in a plateau region in the thermal conductivity data. Furthermore, we derive the phonon mean free path $l = 3\kappa/(C_V v)$, finding an overdamped region for temperatures higher than the corresponding Einstein energies. It is noteworthy that the mean free path in the overdamped region is comparable to phonon wavelengths corresponding to the found Einstein energies.

15 min. coffee break

MM 5: Nanomaterials I: Mechanics

Time: Monday 10:15–11:30

Location: H53

MM 5.1 Mon 10:15 H53

Chemical crosslinking inside an organic/inorganic nanosupercrystal — ●AXEL DREYER¹, ARTUR FELD², ANDREAS KORNOWSKI², EZGI D. YILMAZ¹, HESHMAT NOEI³, ANDREAS MEYER², ANDREAS STIERLE³, HORST WELLER², and GEROLD A. SCHNEIDER¹ — ¹Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe — ²Universität Hamburg, Institut für Physikalische Chemie — ³DESY, NanoLab

Natural hard tissues like nacre are characterized by outstanding mechanical properties. The key to their behavior is the combination of hard inorganic and soft organic constituents on the nanoscale. Our approach is to synthesize a bio-inspired material by self-organization of organic-coated Fe₃O₄ nanoparticles into a well-ordered superstructure. The inorganic particles are separated by a layer of surfactants that is about one nanometer thick. Therefore, the organic molecules

play a prominent role by providing cohesion in the material via strong coordinative bonding of functional groups to the particles surface as well as weak van der Waals bonding between adjacent molecules. To improve the mechanical properties, we substitute the weak van der Waals interaction by strong covalent bonds through thermally induced crosslinking of unsaturated surfactants performed in the solid composite, which yields values of up to 3.4 GPa, 60 GPa, and 630 MPa for microscale hardness, modulus, and strength, respectively. We will discuss which chemical processes take place in the organic phase. This knowledge enables a tailor-made synthesis of surfactants for optimization of the mechanical properties.

MM 5.2 Mon 10:30 H53

Mechanical properties of amorphous/crystalline multilayer structures in the Fe-P system — ●TIMO MÜLLER, ANDREA BACH-

MAIER, MANUEL PFEIFENBERGER, THOMAS SCHÖBERL, and REINHARD PIPPAN — Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Nanolamellar structures of alternating amorphous and crystalline layers are good candidates for combining high strength and ductility due to the combination of the different deformation mechanisms in the two components. In the present study, such structures were prepared in the Fe-P system using electrodeposition. The width of the individual layers was varied from about 250 nm down to a few nanometers. Microhardness testing revealed a Hall-Petch behavior with respect to the layer width for layers larger than 15 nm, whereas an approximately constant hardness of 6.7 GPa was observed for thinner layers. Nanoindentation and micromechanical testing was used to get further insights into the mechanical behavior of these materials.

MM 5.3 Mon 10:45 H53

Modeling the Mechanics of Metallic Nanolattices — ●ALEXANDER STUKOWSKI¹ and BERNHARD EIDEL² — ¹Technische Universität Darmstadt — ²Universität Siegen

Ultralight metallic lattices are a special form of cellular material with structural features on the micron and nanometer scales. Very recent advances in fabrication techniques and several promising applications have sparked great interest in the optimization of such materials and in developing an understanding of the underlying physical mechanisms that determine their stiffness and strength.

Continuum mechanics descriptions alone, however, are unable to describe important small-scale materials phenomena, most notably the transition from nanoelasticity to nanoplasticity. In this contribution we present results from fully atomistic simulations of metallic nanolattices, which have been performed for the first time to investigate the competing elastic and inelastic processes that determine the performance of these structural materials. Our large-scale simulations indicate that the prevailing plastic deformation mechanisms in thin-walled, Ni-based nanolattices is twinning while the deformation of full-profile

lattice structures beyond the elastic regime is carried by dislocations. The extent of the elastic regime is controlled by the shape and architecture of the structures, but also local features such as notches and fillets that can induce or prevent stress concentrations.

MM 5.4 Mon 11:00 H53

Exploiting Electrocapillary Coupling at Metal Surfaces for Active Strain Sensing with Nanoporous Gold —

●CHARLOTTE STENNER¹, LIHUA SHAO², NADIHA MAMEKA³, and JÖRG WEISSMÜLLER^{1,3} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — ²Beijing Institute of Nanoenergy and Nanoscience, Chinese Academy of Sciences, China — ³Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany

We investigate nanoporous gold (NPG) imbibed with electrolyte as a hybrid material, in which the metal acts as an electrode. Due to the large surface-to-volume ratio of NPG the properties of the hybrid material are particularly determined by the metal-electrolyte interface.

An applied strain on NPG is expected to cause measurable potential variations, since the impact of mechanical deformation of a planar gold electrode on its potential is large [1]. Our experiments demonstrate that NPG can be used for sensing elastic strain via measuring either current or potential response of the electrode. The electrochemical signals generated by cyclic straining are robust and sensitive, their magnitude increases with increasing strain amplitude. To connect strain-sensing and actuation measurements on the NPG-based hybrid material, we introduce a theoretical strain-sensing actuation relation that leads to excellent agreement with the experimental results. Thus, one can make predictions about sensing properties using effective actuation parameters and vice versa.

[1] M. Smetanin, Q. Deng and J. Weissmüller, PCCP 13 (2011) 17313

15 min. coffee break

MM 6: Liquid and Amorphous Metals II: Shear bands

Time: Monday 11:30–13:00

Location: H52

MM 6.1 Mon 11:30 H52

Nucleation and propagation of shear bands in metallic and network-forming glasses — ●RICHARD JANA and LARS PASTEWKA — Institut für Angewandte Materialien - Computational Materials Science, Karlsruher Institut für Technologie (KIT), Karlsruhe, Deutschland

Molecular Dynamics simulations (MD) were used to study nucleation and propagation of shear bands during simple shear deformation of CuZr binary bulk metallic glasses (BMG), amorphous silicon (a-Si) and amorphous carbon (a-C). We find that the initial shear bands in a-Si and a-C are more localized than those found in CuZr. Shear bands in a-Si and a-C can be easily morphologically distinguished from their bulk from simple parameters such as the local coordination number and density. While such a clear signature of shear-banding is not found in local topological parameters for CuZr, such as short-range order (SRO) determined by Voronoi tessellation, we show by repeated deformation and quench sequences that in neither case dynamic shear localization through viscous heating and subsequent local softening is the cause of the localization. Nevertheless, thermal effects show impact on the shear localization, as shear bands vanish at elevated temperatures even below T_g . We correlate the temperature-dependence of coordination number and SRO with the evolution of shear banding at elevated temperatures.

MM 6.2 Mon 11:45 H52

Nonlinear Response in Metallic Glasses under Mechanical Excitation — ●BIRTE RIECHERS and KONRAD SAMWER — 1st Physics Department, Georg-August-University Göttingen, Germany

As stress-strain-curves of metallic glasses show, these materials can easily be driven from linear behavior at low mechanical fields to the nonlinear regime by applying comparably high mechanical fields at fixed temperature.

This provides a promising opportunity for investigating the effects of external fields on the relaxation mode spectrum. If the nonlinear regime is entered by using high strains, changes in the shape of the po-

tential energy landscape are expected. This results in a redistribution of relaxation modes and even leads to changes in the shape of the relaxation mode spectrum. MD-simulations on metallic glasses [1,2] have shown this tremendous impact, and predict a transition from fragile to strong behavior.

In this experimental work, the influence of high mechanical strain on the metallic glass $Pd_{40}Ni_{40}P_{20}$ is investigated. The change of the overall relaxation mode spectrum is analyzed with a focus on the behavior of α - and β -processes. Also the redistribution timescale, which is the timescale on which the spectrum equilibrates to a change in external field [3], will be compared to timescales inherent to the relaxation processes of the system.

Financial support by the DFG Research Unit FOR 1394. [1]: H.-B. Yu, Nat. Comm. 6, 2015; [2]: H.-B. Yu, Phys.Rev.B 90, 144201, 2014; [3]: B. Riechers, J. Chem. Phys. 142, 2015;

MM 6.3 Mon 12:00 H52

Physical insights into the mechanisms of tensile creep of a $Pd_{40}Ni_{40}P_{20}$ Bulk Metallic Glass — ●ISABELLE BINKOWSKI¹, SERGIY V. DIVINSKI^{1,2}, and GERHARD WILDE^{1,3} — ¹Institute of Materials' Physics, University of Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — ²National University of Science and Technology "MISIS", Leninsky pr.4, Moscow, Russia — ³Institute of Nanochemistry and Nanobiology, Shanghai University, Shanghai 200072, China

Bulk metallic glasses (BMGs) are known for their high elastic limit, high yield strength, high hardness, corrosion resistance and soft magnetic properties. However, engineering requires a suitable amount of deformability, which, in the case of bulk metallic glasses, is lacking. At sufficiently low temperatures (below T_g) or at high strain rates, deformation of BMGs proceeds inhomogeneously via the formation of thin 2D-like regions of localized strain, so-called shear bands, whose continued activation lead to a catastrophic failure.

For fundamental investigations of properties and mechanisms of shear banding, a $Pd_{40}Ni_{40}P_{20}$ BMG is used, due to its high ther-

mal stability against crystallization in a wide temperature range. A set of miniaturized tensile creep tests is performed at constant stress conditions to give further insights into the shear band events and shear band interactions. The tests are performed in the temperature range between 413 K to 443 K and the stress is fixed at 900 MPa which is about 60% of the yield stress.

A financial support of DFG via SPP 1594 is acknowledged.

MM 6.4 Mon 12:15 H52

Creep of Cu-Zr glass composites studied by Molecular Dynamics simulations — ●CONSTANZE KALCHER, TOBIAS BRINK, ALEXANDER STUKOWSKI, and KARSTEN ALBE — FG Materialmodellierung, FB Materialwissenschaft, Technische Universität Darmstadt, Germany

Over the past two decades, the mechanical properties of metallic glasses have been studied intensively. It is widely accepted that their deformation at low temperature is heterogeneous and that in this regime shear bands can occur. However, when considering high-temperature applications, closer to the glass transition temperature, $T > 0.6T_g$, the possibility of plastic deformation through creep has to be taken into account. In contrast to crystals, where one can clearly distinguish between three different creep stages, the mechanisms behind high-temperature creep behavior of amorphous alloys is still unclear. In this work we compare a homogeneous $\text{Cu}_{64}\text{Zr}_{36}$ glass with glass-crystal (B2 Zr) composites with different topologies: a) interpenetrating network b) rods and c) embedded particles. While the pristine metallic glass deforms homogeneously, the glass-crystal composites form shear transformation zones at the glass/crystal interfaces. Furthermore, we show what influence the topology of the interfaces has on the creep behavior and its activation energy.

MM 6.5 Mon 12:30 H52

A Molecular Dynamics Simulation Study On The Avalanche Dynamics And The Microstructure Evolution Of The Glassy $\text{Cu}_{50}\text{Zr}_{50}$ System. — ●ALEXANDRA LAGOIANNI and KONRAD SAMWER — Erstes Physikalisches Institut, Goettingen, Deutschland

The presence of avalanches/stress drops in the plastic regime of BMGs upon mechanical deformation, and their direct correlation with the formation and arrest of single shear bands [1-2], has been revealed by several experimental studies the last decades. Aiming to gain a deeper insight of this phenomenon on a smaller length scale we employed molecular dynamics simulations of an amorphous CuZr system

under tension. Different strain rates were tested at room and glass transition temperature and the distribution of stress drops sizes was found to follow a power law which exponent is in agreement with that predicted by the avalanche dynamics theory [3]. It came out that the serrated flow takes place even from the very beginning of the elastic region while the possible alterations that occur in the microstructure of the system were exhaustively studied. The present simulation results provide a theoretical confirmation of the experimental findings and a deeper and qualitative understanding of the origin of avalanches in a metallic glass.

[1] Krisponeit, J.O, Pitikaris S., Avila K.E., Küchemann, S., Krüger, Samwer, K. Nature Communications 5, 3616 (2014). [2] Dalla Torre, F.H., Dubach, A., Nelson A., Löffler J.F. Materials Transactions 48, 7, pp. 1774-1780 (2013). [3] Dahmen K.A, Ben-Zion Y., Uhl J.T. Nature Physics 7 pp. 554-557 (2011).

MM 6.6 Mon 12:45 H52

Avalanches upon the deformation process in metallic glasses — ●CARLOS HERRERO-GOMEZ and KONRAD SAMWER — I Physikalisches Institut, Universität Göttingen

Bulk metallic glasses respond with elastic and/or plastic deformation to applied mechanical stresses. Such deformation is not a smooth response to the applied stress but instead take place via jerky jumps, which are often referred as Crackling Noise [1].

We report a statistical analysis of the crackling noise produced by metallic glasses during creep measurements. We present a waiting time analysis of such measurements. Such analysis reveals that the waiting time distribution follows a power law, in the same fashion of simulations and experiments of avalanche dynamics [2,3]. Furthermore, the study shows the existence of a crossover in the waiting times distribution [4]. The crossover was interpreted as a change in the deformation process. We performed a systematic analysis for different experimental conditions, to analyze the influence of the stress and temperature on the avalanche dynamics.

Financial support by the ITN-FP7 Marie Skłodowska-Curie program VitriMetTech N. 607080 is thankfully acknowledged .

[1] K. Dahmen, Y. Ben-Zion and J.T. Uhl. Phys Rev Lett.102, 175501 (2009) [2] M.C: Kuntz, and J.P. Sethna. Phys. Rev. B, 62, 17 (2000) [3] J. Antonaglia, W.J. Wright, X.G. Ru, G.R. Byer, T. C. Huftnagel, M.Lebblanc, J.T.U. and K.A. Dahmen.Phys. Rev. Lett. 112, 155501 (2014) [4] J.O Krisponeit, S. Pitikaris, K.E.Ávila, S.Küchemann, A.Krüger and K. Samwer. Nat. Commun. 5, 3616 (2014)

MM 7: Transport I: Electronic and thermal transport

Time: Monday 11:30–12:45

Location: H53

MM 7.1 Mon 11:30 H53

Non-linear conductance in mesoscopic weakly disordered wires - Interaction and magnetic field asymmetry — CHRISTOPHE TEXIER^{1,2} and ●JOHANNES MITSCHERLING^{1,3} — ¹LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France — ²Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France — ³Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Whereas it is well known that the linear conductance of a two-terminal device is symmetric with respect to magnetic field reversal, the electronic interaction causes an asymmetry of the non-linear conductance $\mathcal{G} \sim \partial^2 I / \partial V^2|_{V=0}$, which can thus be used as a probe of interaction as it was proposed in quantum dots in the ergodic regime [1,2].

We study the non-linear transport in weakly disordered metallic wires in the diffusive regime [3]. The analysis is based on the scattering approach including the effect of electronic interaction (screening) proposed by Büttiker. The dependence of the non-linear conductance in the phase coherence length is determined. The role of thermal fluctuations is also considered.

[1] D. Sánchez and M. Büttiker, Phys. Rev. Lett. 93, 106802 (2004)

[2] B. Spivak and A. Zyuzin, Phys. Rev. Lett. 93, 226801 (2004)

[3] C. Texier and J. Mitscherling, arXiv:1510.02214 (2015)

MM 7.2 Mon 11:45 H53

Evidence for hydrodynamic electron flow in PdCoO₂ — PHILIP

MOLL^{1,2}, PALLAVI KUSHWAHA³, ●NABHANILA NANDI³, BURKHARD SCHMIDT³, and ANDREW MACKENZIE^{3,4} — ¹Laboratory for Solid State Physics, ETH Zurich, Switzerland — ²Department of Physics, University of California, Berkeley, California 94720, USA — ³Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — ⁴Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

The electrical resistance is conventionally determined by the momentum-relaxing scattering of electrons by the host solid and its excitations. Hydrodynamic fluid flow through channels, in contrast, is determined by geometrical factors, boundary scattering and the viscosity of the fluid, which is governed by momentum-conserving internal collisions. A longstanding question in the physics of solids has been whether the viscosity of the electron fluid plays an observable role in determining the resistance. At first sight this seems unlikely, because in almost all known materials the rate of momentum-relaxing collisions dominates that of the momentum-conserving ones that give the viscous term. Here, we show this is not always the case. We report experimental evidence that the resistance of restricted channels of the ultra-pure two-dimensional metal PdCoO₂ has a large viscous contribution. Comparison with theory allows an estimate of the electronic viscosity to be similar to water at room temperature or liquid nitrogen at 75 K.

MM 7.3 Mon 12:00 H53

Hyperfine Interactions in Pd foils during D/H electro-

chemical loading — ●ERIC BERNARDO DA SILVA¹, JULIANA SCHELL^{2,3}, JOÃO G. M. CORREIA^{2,4}, GRAHAM K. HUBLER⁵, VITTORIO VIOLANTE⁶, MOUSTAPHA THIOYE⁷, JINGHAO HE⁵, and MICHEL ZOGHBY⁸ — ¹Instituto de Pesquisas Energéticas e Nucleares, São Paulo University, Brazil — ²ISOLDE-CERN — ³Universität des Saarlandes, Germany — ⁴C2TN, Centro de Ciências e Tecnologias Nucleares, Instituto Superior Técnico, University of Lisbon, Portugal — ⁵Sidney Kimmel Institute for Nuclear Renaissance, Dept. of Physics and Astronomy, University of Missouri, USA — ⁶ENEA, Italian Agency for Energy New Technologies and Sustainable Development, Rome, Italy — ⁷State University of New York, Stony Brook, USA — ⁸Consultant, Thoiry, France

Since 1989, the Fleischmann and Pons Effect (FPE), the appearance of anomalous excess heat (AHE) during electrolytic loading of hydrogen in metal, has been observed, well above measurement uncertainty, in numerous calorimetric experiments. In the present work, Perturbed Angular Correlations (PAC) was used to probe Pd samples, implanted at 80keV with low concentration of radioactive 181Hf (181Ta). During loading of D₂O or H₂O, three different EFG distributions were observed; static, dynamic, and a specific. These EFG distributions, which are only felt by about 10, 15 percent of the Hf/Ta probe atoms and only appear during D loading above 81 percent ($[D]/[Pd]$), could be explained by a temporary atomic rearrangement of D atoms in some zones of the Pd lattice.

MM 7.4 Mon 12:15 H53

Thermal Conductivities in Solids from First Principles: Accurate Computations and Rapid Estimates — ●CHRISTIAN CARBOGNO and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In spite of significant research efforts, a first-principles determination of the thermal conductivity κ at high temperatures has remained elusive. Boltzmann transport techniques that account for anharmonicity perturbatively become inaccurate under such conditions. *Ab initio* molecular dynamics (MD) techniques using the *Green-Kubo* (GK) formalism capture the full anharmonicity, but can become prohibitively costly to converge in time and size. We developed a formalism that accelerates such GK simulations by several orders of magnitude and

that thus enables its application within the limited time and length scales accessible in *ab initio* MD. For this purpose, we determine the *effective* harmonic potential occurring during the MD, the associated temperature-dependent phonon properties and lifetimes. Interpolation in reciprocal and frequency space then allows to extrapolate to the macroscopic scale. For both force-field and *ab initio* MD, we validate this approach by computing κ for Si and ZrO₂, two materials known for their particularly harmonic and anharmonic character. Eventually, we demonstrate how these techniques facilitate reasonable estimates of κ from existing MD calculations at virtually no additional computational cost.

MM 7.5 Mon 12:30 H53

Strain engineering of thermal transport in 2D grain boundaries — ●LEONARDO MEDRANO SANDONAS^{1,2}, RAFAEL GUTIERREZ¹, ALESSANDRO PECCHIA³, GOTTHARD SEIFERT⁴, and GIANAURELIO CUNIBERTI^{1,5,6} — ¹Institute for Materials Science, TU Dresden, Dresden, Germany — ²Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ³Consiglio Nazionale delle Ricerche, ISMN, Rome, Italy — ⁴Physical Chemistry Department, TU Dresden, Dresden, Germany — ⁵Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — ⁶Dresden Center for Computational Materials Science, TU Dresden, Dresden, Germany

Grain boundaries (GBs) in two-dimensional materials have attracted great attention in recent years due to its unique physical properties. However, many questions are still unanswered about the influence of external factors on their thermal properties. Thus, we want to provide some insights in understanding the influence of strain on the thermal transport in 2D materials with grain boundaries. To do this, we employ Green's functions technique combined with DFTB theory. Our main focuses are grain boundaries in novel two-dimensional materials like hBN, Phosphorene, and MoS₂, which are potential candidates for developing novel approaches to nanoscale electronics and phononics. Among the GBs studied in the present work (5|7 and 4|8), 4|8 GB has the stronger influence on the thermal transport. Moreover, we have found an anomalous behavior of the thermal conductance after increasing the uniaxial strain. This trend is associated to the strain dependence of the bond length and the force constants of the material.

MM 8: Topical session: Integrated computational materials engineering for design of new materials II

Time: Monday 11:45–13:15

Location: H38

Topical Talk MM 8.1 Mon 11:45 H38
Modern materials design from first-principles: Recent progress and future prospects — ●BLAZEJ GRABOWSKI — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The ever increasing demand on the performance of modern materials requires optimized design strategies. Experimental techniques alone often reach their limits and need to be supported by atomistic simulations rooted in first-principles. The great challenge is to bridge the gap between quantities accessible by simulation and quantities relevant to experiment. In this talk, I will discuss our recent progress in tackling this challenge and the implications of our work on future research, by focusing in particular on the impact of finite temperatures and microstructural complexity.

MM 8.2 Mon 12:15 H38

Characterization of deformation with various dimensionalities in MoSi₂ — ●MOJMÍR ŠOB^{1,2,3} and MARTIN FRIÁK^{2,1} — ¹Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — ²Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno, Czech Republic — ³Department of Chemistry, Faculty of Sciences, Masaryk University, Brno, Czech Republic

We explore, with the help of *ab initio* electronic structure calculations, the response of molybdenum disilicide (MoSi₂) to a series of extreme applied loading conditions with different dimensionality. Our study is focused on energetics and structural behavior of MoSi₂ with tetragonal C11_b structure under uniaxial, biaxial (epitaxial) and triaxial (hydrostatic) strains and stresses. Total energies and fully relaxed structural parameters are calculated by the Vienna *Ab initio* Simulation Package (VASP) using generalized gradient approximation (GGA). Three

constrained minimum-energy paths corresponding to the uniaxial tensile test simulation along the [001] direction, biaxial stresses within the (001) plane, and triaxial loading conditions are discussed. A relaxation of both external and internal degrees of freedom is performed and their response to the different loading modes is analyzed. Studying the energy vs. strain curves, features common to all three types of strains are analyzed in accordance with the universal binding energy concept.

MM 8.3 Mon 12:30 H38

DFT-simulations of W-Be-alloys for ITER — ●JENS BRÖDER^{1,2}, MARTIN KÖPPEN², DANIEL WORTMANN¹, STEFAN BLÜGEL¹, and CHRISTIAN LINSMEIER² — ¹Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — ²Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

One of the key challenges in the construction of the fusion reactor ITER lies in understanding the evolution of wall materials mostly consisting of W and Be. Here, experiments performing a chemical analysis by interpreting photoelectron spectroscopy spectra are very important. Density functional theory simulations with an all-electron code can assist by relating the measured core-level shift to the chemical environment and therefore support the evaluation of such core-level spectra. Furthermore, the simulated density of states allows the determination of the electronic properties as validated experimentally by valence-band spectroscopy.

In this talk we present calculations of core-level shifts using the FLEUR-code [1]. We use the initial-state approximation and show results for tungsten-beryllium alloys and compare them to experimental findings. In detail, we discuss the surface core-level shifts of relaxed

tungsten surfaces and the chemical shifts of stable W-Be alloys.

We acknowledge financial support in part from MAX (Materials design at the eXascale) Horizon 2020 EINFRA-5.

[1] <http://www.flapw.de>

MM 8.4 Mon 12:45 H38

Sampling free energies of different phases in Fe including atomic and magnetic degrees of freedom — ●MARTIN STAADT¹, JUTTA RO GAL¹, TILMANN HICKEL², JÖRG NEUGEBAUER², and RALF DRAUTZ¹ — ¹Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany — ²Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The phase transition between ferrite and austenite in iron is omnipresent during manufacturing and processing of steels. Due to the combination of a structural and a magnetic transition from paramagnetic FCC to ferromagnetic BCC iron, these phase transitions are particularly challenging to investigate on the atomistic level. Previous studies were limited to embedded atom potentials that did not explicitly account for magnetism or density functional theory that proved to be too computationally expensive for a direct simulation. We overcome these limitations by using bond-order potentials that enable us to treat larger system sizes but still properly treat magnetism. Using the BOPfox code, we calculate free energies of the bulk phases and the phase boundaries with thermodynamic integration including all important contributions.

MM 8.5 Mon 13:00 H38

MM 9: Interfaces II: Segregation and embrittlement

Time: Monday 11:45–12:45

Location: H39

MM 9.1 Mon 11:45 H39

Multiscale modelling of gallium induced embrittlement in aluminium — ●VENKATA SAI PAVAN KUMAR BHOGIREDDY¹, MIRA TODOROVA¹, ROBERT SPATSCHEK^{1,2}, and JÖRG NEUGEBAUER¹ — ¹Max Planck Institut für Eisenforschung, Düsseldorf, Germany — ²Research Center Jülich, Jülich, Germany

Liquid metal embrittlement is a degradation phenomenon in which a solid metal undergoes brittle failure when it is stressed while in contact with a liquid metal. The transition from ductile to brittle metal failure manifests itself by rapid crack propagation which reduces the elongation to failure ratio.

Combining density functional theory calculations with continuum methods, we study the liquid metal embrittlement of aluminium in contact with gallium. Comparing *ab-initio* calculated energies for a $\Sigma 3$ and a $\Sigma 5$ Al grain boundary and their corresponding surface energies in the presence and absence of Ga, we identify critical Ga concentrations which result in a weakening of the mechanical strength of aluminium.

Parametrising the DFT results in continuum model we obtain the concentration as a function of the strain in the system. In a final step we extend this approach and compute the stress field induced by cracks in bulk and at grain boundaries. The stress field explains the large segregation of gallium atoms at the crack tip and the crack tip's subsequent propagation.

MM 9.2 Mon 12:00 H39

Chemical trends in grain-boundary elasticity from *ab initio* calculations: case study of $\Sigma 5(210)$ Ni₃(Al,Si) — ●MARTIN FRIÁK^{1,2}, MONIKA VŠIANSKÁ^{2,1}, DAVID HOLEC³, and MOJMÍR ŠOB^{2,1,4} — ¹Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — ²Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — ³Montanuniversität Leoben, Leoben, Austria — ⁴Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We employ quantum-mechanical calculations within the density functional theory to study elastic properties of $\Sigma 5(210)$ grain boundaries (GB) in Ni₃Al with and without segregated Si atoms substituting Al atoms. Anisotropic elastic properties of 64-atom computational supercells (as periodic approximants of GBs) are determined using the stress-strain method. We compare elastic properties of two chemical compositions of the $\Sigma 5(210)$ GB in Ni₃Al with those with Si atoms at different Al positions at this GB. The elastic properties of the $\Sigma 5(210)$ GB Ni₃Al grain boundaries are found to be very different from the

Thermal properties of paramagnetic α -Mn from first principles — ●HOSSEIN EHTESHAMI and PAVEL A. KORZHAVYI — Materials Technology, Department of Materials Science and Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Mn is a common alloying element in steel. Therefore, its physical properties and their variation with temperature are of interest for thermodynamic modeling. α -Mn is a complex cubic phase that is stable between 0 and 1000 K and undergoes antiferromagnetic ordering below the Neel point of about 100 K. For an element with such complex crystal and magnetic structures, one can expect that the magnetic, electronic and vibrational degrees of freedom are coupled. Here we describe the paramagnetic phase of α -Mn at finite temperatures by decoupling adiabatically the "fast" (electronic and magnetic) and "slow" (vibrational) degrees of freedom. The electronic structure is calculated within the exact muffin-tin orbital (EMTO) formalism. Electronic excitations are included via finite-temperature smearing of the Fermi function. Paramagnetic disorder is treated self-consistently in the disordered local moment (DLM) model and coherent potential approximation (CPA). The so obtained partial free energies (including the electronic and magnetic contributions as functions of temperature and volume) are used as the input to the Debye-Grüneisen model of the lattice vibrations. Thermal expansion, isothermal/adiabatic bulk modulus and specific heat capacities are calculated and compared with the experimental results to demonstrate the validity of the adiabatic treatment.

bulk (they possess orthorhombic symmetry and are softer) and exhibit high sensitivity to the chemistry of the grain-boundary interface and its surrounding atomic neighborhood. This sensitivity is, nevertheless, limited to only a few atomic layers away from the grain boundary. Comparing our quantum-mechanical results with predictions obtained by linear-elasticity approach we demonstrate deficiencies of the latter and thus a clear need to use *ab initio* methods in this field.

MM 9.3 Mon 12:15 H39

Hydrogen behaviour at structural defects in high-strength steels — ●EUNAN J. MCENIRY, TILMANN HICKEL, and JÖRG NEUGEBAUER — Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The behaviour of hydrogen in high-strength steels is well-known to play a very significant role in the long-term stability and mechanical properties of such materials. Experimental and theoretical work has indicated that structural defects, such as grain boundaries, dislocations, nanovoids and phase boundaries between the matrix and precipitates present in the material, play the most important role in the phenomenon of hydrogen embrittlement.

Using atomistic simulations, we have examined the energetics and diffusion of hydrogen in the vicinity of such extended defects. Particular emphasis has been placed on a wide range of grain boundaries in ferrite, and on semi-coherent interfaces between ferrite and non-metallic inclusions such as TiC and TiN. Due to the large system sizes required to simulate, for example, low-symmetry grain boundaries or misfit dislocations between the matrix and inclusions, conventional *ab initio* simulations are no longer feasible. In this direction, we have developed scale-bridging atomistic potentials based on the tight-binding approximation, which still allow for a fully quantum-mechanical treatment of the system.

MM 9.4 Mon 12:30 H39

Effect of Sb segregation on conductance and catalytic activity at Pt/Sb-doped SnO₂ interface: a synergetic computational and experimental study — QIANG FU^{1,5}, LUIS CÉSAR COLMENARES RAUSSE², ●UMBERTO MARTINEZ POZZONI³, PAUL INGE DAHL², JUAN MARIA GARCÍA LASTRA¹, PER ERIK VULLUM^{2,4}, INGEBORG-HELENE SVENUM^{2,4}, and TEJS VEGGE¹ — ¹Department of Energy Conversion and Storage, Technical University of Denmark, Lyngby, Denmark — ²SINTEF Materials and Chemistry, Trondheim, Norway — ³QuantumWise A/S, Copenhagen, Denmark —

⁴Department of Physics, Norwegian University of Science and Technology (NTNU) Trondheim, Norway — ⁵Current Address: Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

In this work, the effect of Sb segregation on the conductance and catalytic activity at Pt/Antimony doped tin dioxide (ATO) interface was investigated through a combined computational and experimental study. It was found that Sb-dopant atoms prefer to segregate toward

the ATO/Pt interface. The deposited Pt catalysts, interestingly, not only promote Sb segregation, but also suppress the occurrence of Sb³⁺ species, a charge carrier neutralizer at the interface. The conductivity of ATO was found to increase, to a magnitude close to that of activated carbon, with an increment of Sb concentration before reaching a saturation point around 10%, and then decrease, indicating that Sb enrichment at the ATO surface may not always favor an increment of the electric current.

MM 10: SYCE: Caloric effects in ferroic materials

Time: Monday 15:00–17:45

Location: H1

Invited Talk

MM 10.1 Mon 15:00 H1

Multicaloric effects in metamagnetic Heusler materials — ●ANTONI PLANES — Departament d'Estructura i Constituents de la Matèria. Facultat de Física. Universitat de Barcelona. Diagonal 647. 08028 Barcelona. Catalonia.

The talk is aimed at presenting a general thermodynamic framework to deal with multicaloric effects in multiferroic materials. After discussing a number of recently reported examples showing that various caloric effects may occur in the same material interdependently, the formalism will be applied to the study of multicaloric effects taking place near the magnetostructural transition in metamagnetic Heusler shape-memory materials. This class of metamagnetic materials will be modelled by means of a Landau free energy expansion with appropriate interplay between the corresponding structural and magnetic order parameters. Caloric effects will be quantified by the isothermal entropy changes and the adiabatic temperature changes induced by application of the fields thermodynamically conjugated to the order parameters. It will be shown that multicaloric effects comprise the corresponding contributions from the effects associated with each ferroic property and the cross-contribution arising from the interplay between these properties. Finally, the obtained results will be compared with available experimental data.

Invited Talk

MM 10.2 Mon 15:30 H1

Multicaloric effect in biological systems: a case of nerve action — ●MATJAZ VALANT¹, LAWRENCE J. DUNNE², ANNA-KARIN AXELSSON², FLORIAN LE GOUPL³, and GEORGE MANOS⁴ — ¹University of Nova Gorica — ²London South Bank University, UK — ³Imperial College London, UK — ⁴University College London, UK

In the recent decades the "caloric community" has demonstrated the technological value of different types of reversible caloric effects induced by pulsing external fields that trigger changes in materials* order parameters. The applied research continues towards first prototypes of refrigeration systems. In addition, we have gained much better understanding of the microscopic processes related to the caloric effects, which enabled us also to recognize their occurrence and role in biological systems. We will discuss a model of nerve action, which is a natural continuation of the solitonic model that considers a solitonic type pressure/density pulse propagating along the long axis of the nerve. A special emphasis has been placed on a reversible caloric response during the nerve action, which can be described as a multicaloric effect. We have calculated changes in membrane temperature, thickness, entropy and trans-membrane voltage. All of these calculated parameters are in striking agreement with experimental results. The temperature change is explained with the solitonic propagation that is iso-entropic. This observation is an important biological manifestation of the multicaloric effect, which has hitherto not being described in these terms.

Invited Talk

MM 10.3 Mon 16:00 H1

Optimizing the electrocaloric effect by first-principles simulations: The role of strain and defects — ●ANNA GRÜNEBOHM — University of Duisburg-Essen and Cenide, Germany

The electrocaloric effect (ECE) is the adiabatic temperature change of a material in a varying external electrical field. The ECE is promising for novel cooling devices [1]. However, in many ferroelectrics the large ECE is restricted to a narrow temperature interval.

To model modifications of the ferroelectric and electrocaloric properties of BaTiO₃ by defects and epitaxial strain we have combined *ab initio*-based molecular dynamics simulations with a simple model for defects [2]. For polar defects the temperature range of the large caloric response is broadened. Still more striking, a giant inverse caloric effect

has been observed for the first time.

Additionally, epitaxial strain can be used to enhance the caloric response and shift the operation range [3,4]. In particular tensile strain is promising to enhance the ECE of BaTiO₃ around room temperature.

[1] X. Moya, *et al.*, *Nature Mater.* **13**,439 (2014)

[2] A. Grünebohm, *et al.*, arXiv:1502.05201

[3] M. Marathe, *et al.*, *APL* **104**, 212902 (2014)

[4] A. Grünebohm, *et al.*, *APL* **107**, 102901 (2015).

15 min. coffee break

Invited Talk

MM 10.4 Mon 16:45 H1

Giant inverse barocaloric effects in ferrielectric ammonium sulphate — POL LLOVERAS¹, ENRIC STERN-TAULATS², MARIA BARRIO¹, JOSEP LLUIS TAMARIT¹, SAM CROSSLEY³, WEI LI³, VLADIMIR POMJAKUSHIN⁴, ANTONI PLANES², LLUIS MAÑOSA², NEIL MATHUR³, and ●XAVIER MOYA³ — ¹Departament de Física i Enginyeria Nuclear, ETSEIB, Universitat Politècnica de Catalunya, Diagonal 647, Barcelona, 08028 Catalonia, Spain — ²Facultat de Física, Departament d'Estructura i Constituents de la Matèria, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Catalonia, Spain — ³Department of Materials Science, University of Cambridge, Cambridge, CB3 0FS, UK — ⁴Paul Scherrer Institute, WHGA/133, 5232 Villigen - PSI, Switzerland

Giant barocaloric effects driven by hydrostatic pressure have been suggested for cooling applications, but they are only seen in a small range of magnetic materials that are relatively expensive. Here I will present pressure-dependent calorimetry data to demonstrate giant inverse barocaloric effects in ferrielectric ammonium sulphate, which is made of cheap abundant elements [Lloveras et al., *Nature Communications*, in press].

Invited Talk

MM 10.5 Mon 17:15 H1

TiNiCu-based thin films for elastocaloric cooling — ●ECKHARD QUANDT and CHRISTOPH CHLUBA — Chair of Inorganic Functional Materials, Institute for Materials Science, Faculty of Engineering, University of Kiel, Germany

The elastocaloric effect is a promising alternative for the replacement of conventional vapor compression cooling which suffers from a high environmental impact and limited efficiency improvement possibilities. Instead of a vapor-liquid transition in a conventional cooling, the elastocaloric effect is based on a stress induced structural phase transition usually from a high symmetry to a low symmetry phase. At adiabatic conditions this results in a temperature change of the material. For a continuous use of this effect in a cooling cycle, several requirements have to be fulfilled. Transformation temperatures, effect size and efficiency have to be suitable, but most importantly a high functional and structural fatigue resistance is necessary.

Highly fatigue resistant Ti-rich TiNiCu compositions prepared by thin film technology have been found that can withstand 10 million transformation cycles without functional degradation [1]. Within this talk the reasons for the fatigue resistance will be discussed. In situ synchrotron and TEM investigations have been conducted to investigate the underlying microstructural mechanisms that ensure the reversible transformation. Cobalt and iron addition is used to adjust the transformation temperature to a suitable range to enable the use of this compositions at room temperature. The compositional influence on the elastocaloric parameters is investigated by temperature dependent tensile tests, infrared (IR) thermography and differential scanning calorimetry. Due to the small hysteresis of TiNiCu-based compositions an improved elastocaloric cooling efficiency is found in comparison to

binary NiTi thin films. Considering also the high fatigue resistance, this class of materials is promising for future elastocaloric cooling applications.

[1] Chluba, C.; Ge, W.; Lima de Miranda, R.; Strobel, J.; Kienle, L.;

Quandt, E.; Wuttig, M.: Ultralow-fatigue shape memory alloy films, *Science* 348 (2015), 1004-1007.

MM 11: Topical session: Integrated computational materials engineering for design of new materials III

Time: Monday 15:45–18:00

Location: H39

Topical Talk MM 11.1 Mon 15:45 H39
Search for substitutes of magnetic materials containing critical elements by high-throughput screening and multi-scale modeling — ●CHRISTIAN ELSÄSSER, WOLFGANG KÖRNER, GEORG KRUGEL, MATOUS MROVEC, DANIEL F. URBAN, and PETER GUMB-SCH — Fraunhofer IWM, Freiburg, Germany

This lecture will discuss how new magnetic materials can be discovered by computational high-throughput-screening and multi-scale-modeling approaches, to substitute established magnets like Nd₂Fe₁₄B, which have outstanding functionalities but also constraining criticalities.

A combinatorial high-throughput-screening approach based on density functional theory (DFT) is employed to search for intermetallic phases with crystal structures and chemical compositions, which have good intrinsic ferromagnetic properties but contain no or less amounts of critical rare-earth elements like Nd in Nd₂Fe₁₄B.

To develop magnets from promising magnetic phases requires efficient scale-bridging approaches which take into account how the microstructure influences the magnetic behavior. The size of atomistic models can be increased by tight-binding total-energy and bond-order-potential methods, which are based on DFT and capable to describe extended defects like grain boundaries or lattice dislocations.

A route to magnetic multi-domains and poly-crystals is provided by phenomenological approaches like micro-magnetic or phase-field models, which can be parameterized as well using data bases of materials properties obtained from the atomic level. The lecture will close with an outlook in this direction.

MM 11.2 Mon 16:15 H39
Ab initio analysis of the phase stability of Ce-based hard-magnetic materials — ●HALIL IBRAHIM SÖZEN, TILMANN HICKEL, and JÖRG NEUGEBAUER — The Max-Planck-Institut für Eisenforschung GmbH Max-Planck-Straße 1, 40237 Düsseldorf

In recent years, the development in electro-mobility, i.e. the progressive replacement of oil-based fuels in the transportation by electric motors, increased the demand of hard magnetic materials, which are composed of rare-earths (RE) and transition metals (TM). Recently, there are attempts to develop alternative hard magnets that lift the dependence on the small number of RE elements. For this purpose, ab initio high-throughput calculations have been performed with the focus on a few selected magnetic parameters. However, the decisive question of the phase stability of potential material systems is much less investigated. For example, for Ce-based alloys the magnetically interesting CeFe₁₁Ti phase is thermodynamically competing with a CeFe₂ phase. In order to predict phase stability, we perform ab initio calculations for the Helmholtz free energy $F(T,V)$ taking vibrational, electronic, magnetic and configurational entropy contributions into account. We carefully investigate the performance of density functional theory (DFT) and its extensions to achieve these results and compare the results with Nd-based hard-magnetic materials. Based on these results we provide suggestions as to how the favourable magnetic phases can be stabilized.

MM 11.3 Mon 16:30 H39
Theoretical screening of 1-12 and 1-12-X phases on the search for new hard-magnetic compounds with low rare-earth content — WOLFGANG KÖRNER, ●GEORG KRUGEL, DANIEL F. URBAN und CHRISTIAN ELSÄSSER — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

The ThMn₁₂-type crystal structure recently attracted renewed experimental and theoretical interest as being a promising starting point in the search for new hard-magnetic compounds with low rare-earth content. This is mainly due to the atomic rare-earth to transition-metal ratio of 1:12 and the tetragonal crystal symmetry which is necessary for high magnetocrystalline anisotropy. Estimates of the energy pro-

duct $(BH)_{max}$ for NdFe₁₂N yield about 686 kJ/m³ which even exceeds the best available hard magnet nowadays, namely Nd₂Fe₁₄B with $(BH)_{max}=516$ kJ/m³.

We report on theoretical investigations, by means of density functional theory, of the 1-12 and 1-12-X phases derived from the known ThMn₁₂-type structure. We have extended our computational high-throughput screening (HTS) approach [1] by approximate evaluations of the anisotropy constant K_1 , the anisotropy field H_a and an estimate of $(BH)_{max}$. Our calculation of K_1 is fast since it is based on the crystal field parameters and avoids expensive total-energy calculations. Besides NdFe₁₂N which has the highest magnetization, several 1-12 and 1-12-X compounds based on Ce instead of Nd are presented which are interesting alternative hard-magnetic compounds.

[1] N. Drebov et al, *New J. of Phys.* 15, 125023 (2013)

15 min. coffee break

MM 11.4 Mon 17:00 H39
First-principles study of the colour and reflectivity of metals — ●GIANLUCA PRANDINI^{1,2} and NICOLA MARZARI^{1,2} — ¹THEOS, EPF Lausanne, Switzerland — ²NCCR MARVEL, EPF Lausanne, Switzerland

Gold and copper are the only two elemental metals to show a characteristic colour due to the presence of a drop of the reflectivity curve in the visible range. Reflectivities of all other metals are in general high and flat for all visible frequencies, making them appear shiny and silvery white. Nowadays, with state-of-the-art theoretical methods, it is possible to calculate colour and reflectivity of a material by means of first-principles simulations and, as a practical consequence, predict or design the colour of new alloys. I will show and discuss the results obtained for the reflectivity and colour of elemental metals and of some simple metallic binary alloys. The approach followed for the calculation of the dielectric function is the random-phase approximation (RPA) starting from band structures obtained at the density functional theory (DFT) level using the computationally inexpensive PBE exchange-correlation functional. These results are important in order to establish the computational framework for high-throughput screening of the optical properties of novel metallic alloys.

MM 11.5 Mon 17:15 H39
"Treasure maps" for magnetic CoFeNiCr-based high-entropy-alloys from first-principles — ●FRITZ KÖRMANN¹, DU-ANCHENG MA², DUSTIN BELYEA³, MATTHEW LUCAS⁴, CASEY MILLER³, BLAZEJ GRABOWSKI², and MARCEL SLUITER¹ — ¹Materials Science and Engineering, TU Delft, Delft, Netherlands — ²Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ³Materials Science, Rochester Institute of Technology, Rochester, NY, United States — ⁴Air Force Research Lab, Wright-Patterson AFB, OH, United States

We present finite-temperature magnetic properties of FCC CoFeNiCr-based high entropy alloys (HEA). Particular emphasis is put on CoCr-FeNiPd HEAs, which have T_C s in the neighborhood of ambient [1]. T_C s are computed employing density functional theory and a magnetic mean-field model [2]. Our theoretical results are in excellent agreement with experimental data revealing high predictive power of the employed theoretical method. The computational framework is used to explore the dominant mechanisms that determine T_C . Finally we propose alternative alloying strategies for tuning T_C towards room temperature. Our predicted "treasure maps" [2] narrow down the enormous configuration space for distinct magnetic properties of these multi-component alloys to a well-defined set of alloy compositions revealing a wide range of ferromagnetic properties and T_C s near room temperature in hitherto unexplored alloys. [1] Belyea *et al.*, *Sci. Rep.* 5, 15755 (2015); Lucas *et al.*, *J. Appl. Phys.* 109, 07E307 (2011). [2]

Körmann *et al.*, Appl. Phys. Lett. 107, 142404 (2015).

MM 11.6 Mon 17:30 H39

Ab initio prediction of sound velocities in planetary inner cores — ●JAN W. JAEKEN¹, ATTILIO RIVOLDINI², TIM VAN HOOLST², VERONIQUE VAN SPEYBROECK¹, MICHEL WAROQUIER¹, and STEFAAN COTTENIER^{1,3} — ¹Center for Molecular Modeling, Ghent University — ²Reference Systems and Planetology, Royal Observatory of Belgium — ³Department of Materials Science and Engineering, Ghent University

Earth's inner core's sound velocities and acoustic anisotropy are well known through seismological observation. However, explaining this anisotropy has proven to be difficult. High pressure experiments are not easy to perform, especially when considering exoplanets with even higher core pressures.

Ab initio modeling provides a tool for determining material properties when experiments are difficult or dangerous. We have studied the effect of stacking faults on the sound velocities of close-packed iron at high pressures. We show how the stacking sequence has a crucial effect on acoustic anisotropy.

The method outlined in this work is material-independent, making it a potentially valuable tool in the design of new materials with user-defined sound propagation properties.

MM 11.7 Mon 17:45 H39

MM 12: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Time: Monday 15:45–17:45

Location: H51

MM 12.1 Mon 15:45 H51

Mechanism of Li intercalation/deintercalation into/from the surface of LiCoO₂ — ●ASHKAN MORADABADI and PAYAM KAGHAZCHI — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

LiCoO₂ is the most commonly used cathode material in Li-ion batteries. In this work, we have investigated atomic and electronic structures, magnetic properties, formation energies, and energy barriers for the diffusion of Li in single vacancies, divacancies, and missing rows in bulk and surface of LiCoO₂. Our GGA-PBE results indicate that there is almost no energy barrier for the Li-ion deintercalation from the surface layer. Energy barrier for the Li-ion intercalation is also very small. However, we find that Li hopping in PBE+U is accompanied by electron hopping between nearby transition metal ions. Therefore a PBE+U barrier, which is for both Li hopping and charge hopping, is higher than the corresponding PBE barrier [1]. This study has implications in understanding the role of the surface in the rate capability of nanostructured LiCoO₂ cathodes of Li-ion batteries.

[1] Ashkan Moradabadi and Payam Kaghazchi, Mechanism of Li intercalation/deintercalation into/from the surface of LiCoO₂, Phys. Chem. Chem. Phys., 2015, 17, 22917-22922.

MM 12.2 Mon 16:00 H51

Potential-dependent mechanism of Li diffusion in Li₂S — ●ASHKAN MORADABADI^{1,2} and PAYAM KAGHAZCHI¹ — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — ²Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Li-S batteries are promising candidates for large-scale applications such as electrical vehicles. However, the measured discharge capacity is often less than the theoretical one [1,2]. This is mainly due to the slow diffusion of Li through Li₂S shells formed on S₈ cores, which leads to an incomplete conversion of S₈ cores to Li₂S (the final product of lithiation of S₈). In the present work, using density functional calculation, we have investigated mechanism of Li diffusion in Li₂S. At low cell voltages (< 0.93 V), Li diffusion occurs via an exchange mechanism with a high energy barrier of 0.45 eV. However at higher cell voltages, Li diffusion takes place via a vacancy mechanism with a lower energy barrier of 0.27 eV. Our findings can explain the capacity fading in Li-S batteries at high operation rates.

[1] Liang, X.; Hart, C.; Pang, Q.; Garsuch, A.; Weiss, T.; Nazar, L. F.; A highly efficient polysulfide mediator for lithium-sulfur batteries. Nature Communications, 2015, 6, 5682.

[2] Wang, L.; Wang, Y.; Xia, Y.; A high performance lithium-ion

Ab initio study on GaP-Si interface formation and properties — ●ANDREAS STEGMÜLLER and RALF TONNER — Fachbereich Chemie, Philipps-Universität, 35032 Marburg

In thin-film heterostructures, interfaces determine charge carrier transport and exciton trapping. Here, the GaP-Si interface was chosen as a model system to study the interface formation and associated properties eminent for constructing optoelectronic applications. Experimental findings are reported showing GaP-Si is neither flat nor abrupt but intermixed within 8 atomic layers and faceted.[1]

Abrupt and intermixed interfaces at (001), (111), (112) and (113) are discussed and absolute formation energies from DFT applying large slab- and bulk-type supercells are presented. We separately analyzed local and cell-wide (3-5 nm) features on the atomic structure (local stress vs. material strain), atomic charges (interface charge vs. bulk-like atomic polarization (NPA)), electrostatic potential (transition and convergence through an interface vs. III/V film polarization/oscillating field) and relate them to stability. However, as the materials should be considered covalent (not ionic) and dominated by local contributions, more chemically motivated arguments (e.g. electronegativity) are needed in order to see why simple, charge-based models [2,3] are only qualitatively correct.

[1] Andreas Beyer et al., submitted 2015.

[2] Walter A. Harrison et al., Phys. Rev. B, 18, 4402-4410, 1978.

[3] M. D. Pashley, Phys. Rev. B, 40, 10481-10487, 1989.

sulfur battery based on a Li₂S cathode using a dual-phase electrolyte. Energy Environ. Sci. 2015, 8, 1551.

MM 12.3 Mon 16:15 H51

Extremely high magnetoresistance in topological insulator candidate LaBi — ●NITESH KUMAR, CHANDRA SHEKHAR, and CLAUDIA FELSER — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Lanthanum monpnictides (LaX, X=N, P, As, Sb, Bi) have recently been predicted to be topological insulators, except LaN which is a topological semimetal. Inspired from this report we have studied the transport properties of LaBi. It has a simple rock salt-type structure with alternate La and Bi atoms arranged in all three directions. Temperature variation of resistivity at different magnetic fields follows Kohler's rule. Resistivity follows almost a parabolic relation with magnetic field without saturation, exhibiting a huge magnetoresistance (1.5 x10⁵% at 2 K and 9 T). By employing two band model we calculate carrier density and mobility of electrons and holes which suggests that LaBi is a compensated system. We believe this to be responsible for high unsaturated MR in LaBi. We observe excellent Shubnikov-de Haas (SdH) oscillations starting from around 3T. We also analyse the angle and temperature dependence of these oscillations.

MM 12.4 Mon 16:30 H51

VOTCA-STP - Multi Scale Modeling of Spin Transport in Organic Semiconductors — ●ERIK R. MCNELLIS, SHAYAN HEMMATIYAN, AMAURY MELO SOUZA, SEBASTIAN MÜLLER, and JAIRO SINOVA — Johannes Gutenberg University, Mainz, Germany

Organic molecules present a range of unique and highly attractive properties in solid state technology applications. So also in spintronics, where the weak but highly tailorable spin-orbit coupling in light elements offers spin lifetimes of unparalleled length and controllability.

1st-principles theoretical modeling stands to provide a crucial perspective on the emerging field of spin transport in organic semiconductors. Comprehensive modeling of relevant systems is challenging, with several of the spin transport mechanisms in traditional solid state materials non-existent or strongly modified in organics.

We are developing a multi-scale modeling framework for spin transport in bulk organic materials, based on the VOTCA toolkit for charge transport in the same. The core component is a semi-classical kinetic Monte-Carlo model, with input parameters calculated using 1st-principles theory.

The scope, capabilities of and particular challenges for this development will be presented along with possible extensions to e.g. 'spinterfaces', where spin currents are manipulated by tailoring of an inorganic

/ organic solid interface, as well as a perspective on the potential ramifications for experimental work in the field.

15 min. coffee break

MM 12.5 Mon 17:00 H51

High-pressure and nonlinear elastic response of solids: Example of carbon allotropes — ●PASQUALE PAVONE, ROSTAM GOLESORKHTABAR, STEFAN KONTUR, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

As prototype materials showing strong nonlinear elastic behaviour, diamond and, more recently, layered carbon allotropes have attracted much attention. However, even the nonlinear elasticity of diamond is not completely clarified: Experimentally, nonlinear elastic constants of diamond were investigated only recently [1], showing significant discrepancies with theoretical results. Furthermore, the standard *ab initio* reference calculation for diamond [2] is nowadays about 30 years old and needs to be updated in the light of current development of theory, numerical algorithms, and available computer power. Using the full-potential all-electron package **exciting** [3], we perform a systematic *ab-initio* investigation of the nonlinear elastic properties of diamond, graphene monolayers, as well as simple-hexagonal and hexagonal graphite. We develop an extension of the **ElaStic** tool [4] for the determination of third-order elastic constants. From these results the pressure dependence of linear elastic constants is obtained and connected to dynamical quantities like the mode Grüneisen parameters.

[1] J.M. Lang *et al.*, Phys. Rev. Lett. **106**, 125502 (2011).

[2] O.H. Nielsen, Phys. Rev. B **34**, 5808 (1986).

[3] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).

[4] R. Golezorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).

MM 12.6 Mon 17:15 H51

Calculations of temperature dependent resistivity for transition metals from the first principles — ●DAVID WAGENKNECHT^{1,2}, ILJA TUREK^{1,2}, and KAREL CARVA¹ — ¹Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague; Ke Karlovu 3, 12116 Prague 2, Czech Republic — ²Institute of Physics of Materials, Academy of Sciences of the Czech Republic; Žitkova 22, 61662 Brno, Czech Republic

The temperature dependence of electrical resistivity is studied from

the first principles. Properties of late transition metals have been calculated using the linear muffin-tin orbital (LMTO) method with the coherent potential approximation (CPA). The influence of non-zero temperature has been described by a frozen lattice disorder – atoms were moved from the positions on an ideal lattice and different temperatures are then given by the magnitudes of the random displacement vectors. Dependence of the physical quantities on the parameters of the displacements (like random and non-random directions of the displacement vectors) has been observed and taken into account during discussion of the results. Special attention has been paid to an influence of spin-orbit interaction on the final resistivity, as well as to comparison with other *ab initio* calculations and experimental data; the obtained results agree reasonably well with those of other authors. Derived analytical modifications of the LMTO potential functions and the numerical codes can be now used to calculate relevant physical properties of different materials.

MM 12.7 Mon 17:30 H51

Ab Initio Molecular Dynamics Study of Conjugated Polymer Systems: The Elusive Localization of the Polaron — ●HÅKAN W. HUGOSSON¹, AMINA MIRSAKIYEVA¹, and ANNA DELIN^{1,2} — ¹Department of Materials och Nano Physics, KTH Royal Institute of Technology, Stockholm, Sweden. — ²Ångstrom Laboratory, Uppsala University, Uppsala, Sweden.

The thermoelectric conjugated polymer poly(3,4-ethylenedioxythiophene), or PEDOT, contains a carbon backbone consisting of alternating short and long carbon bonds. Therefore there are two isomeric states: aromatic and quinoid. Charge injection or the presence of charged doping agents leads to the formation of localized charge in the conjugated polymer – a so-called polaron. This polaron induces a localized structural distortion (a shift from the aromatic form towards the quinoid) in the conjugated carbon backbone.

Self-localized polarons in conjugated carbon systems have been found using semi-empirical or HF-theory, but formerly never using DFT with local or gradient corrected functionals (e.g. LDA/BLYP). Self-localization has been seen using DFT and long range hybrid functionals with partial exact exchange included.

Using modern *ab initio* molecular dynamics methods based on DFT we have studied PEDOT and its charge carrying polarons. A localized polaron is now found when studying the time-averaged changes in bond-distances and also in snap-shots for the frontier orbitals for long oligomers (12 monomers).

MM 13: Liquid and Amorphous Metals III: Mechanical properties

Time: Monday 15:45–17:30

Location: H52

MM 13.1 Mon 15:45 H52

Thermal relaxation of metallic glasses: Influence on mechanical properties and structure studied by molecular dynamics simulations — ●TOBIAS BRINK and KARSTEN ALBE — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Metallic glasses show a transition from homogeneous deformation to shear banding depending on temperature and strain rate, with shear banding being the typical mechanism at ambient conditions. The critical values for the transition are determined by the glass composition but should also depend on the structure of the glass. We use molecular dynamics computer simulations to investigate the deformation mechanism in as-quenched and annealed Cu₆₄Zr₃₆ metallic glasses. Due to the very high strain rates in the simulation, the as-quenched glass only exhibits shear banding at low temperatures. In contrast, shear banding occurs at the same strain rates well above room temperature in samples that were annealed for several hundred nanoseconds near T_g . Additionally, properties like structure, short-range order, potential energy, free volume, and vibrational properties (boson peak) change with annealing time, indicating a more relaxed metallic glass, i.e., a decreased fictive temperature. We discuss the shear banding at elevated temperatures in terms of these structure-related changes. Furthermore, we investigate the influence of thermal relaxation on pre-existing shear bands and compare their structural relaxation to that of the matrix.

MM 13.2 Mon 16:00 H52

Ductility changes in the bulk metallic glass former PdNiP due to micro-alloying by adding Cobalt and Iron — ●NIKLAS NOLLMANN, ISABELLE BINKOWSKI, HARALD RÖSNER, and GERHARD WILDE — Universität Münster

Deformation of bulk metallic glasses (BMGs) at low temperatures and high stresses lead to an inhomogeneous plastic flow. During plastic deformation, bulk metallic glasses show almost no ductility and fail alongside shear bands where the strain is localized. This limited ductility has led to substantial effort in order to improve the plasticity of BMGs. We investigated PdNiP based glasses which feature a rather high ductility in bending, compared to other bulk metallic glasses. By the use of micro alloying, the mechanical properties of metallic glasses can be influenced. Adding Iron or Cobalt to the PdNiP BMG leads to a huge change in ductility. To investigate the reason for these changes, the Poisson's ratios were determined by ultrasonic measurements. Interestingly, the plasticity is not reflected by the high Poisson ratio, which remained unaffected by microalloying within the accuracy of the measurement. While analyzing the dependence of the ductility of the present glasses on relaxation treatments, we utilize the fictive temperature concept to investigate the impact of minor alloying on the relative amount of free volume. Also the critical fictive temperature was measured to characterize the ductility of the new BMGs.

MM 13.3 Mon 16:15 H52

Synthesis and Mechanical properties of Cu-Zr metallic Nanoglasses — ●SREE HARSHA NANDAM¹, RUTH SCHWAIGER², JULIA IVANISENKO¹, XIAOKE MU¹, and HORST HAHN^{1,3} — ¹Institute

for Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany. — ²Institute for Applied Materials, Karlsruhe Institute of Technology, D-76344, Eggenstein-Leopoldshafen, Germany. — ³KIT-TUD Joint Research Laboratory Nanomaterials, Institute of Materials Science, Technische Universität Darmstadt (TUD), Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany.

Bulk Cu₅₀Zr₅₀ metallic nanoglass (NG) specimens were synthesized using a modified Inert Gas Condensation method fitted with magnetron sputtering instead of thermal evaporation of the starting alloy. As-sputtered powder had a particle size of about 5-8 nm as observed in a transmission electron microscope. X-ray diffraction of the synthesized pellet confirmed its amorphous nature and energy dispersive spectroscopy showed the equiatomic Cu₅₀Zr₅₀ alloy. Differential scanning calorimetry revealed a crystallization temperature of the NG specimen of around 475°C. Vickers microhardness and compression tests of NG Cu₅₀Zr₅₀ specimens were performed. Similar tests were also carried out on metallic glass ribbons of a similar composition. In order to compare elastic modulus of the nanoglass samples and of the melt spun ribbons, nanoindentation tests were performed. Possible reasons for the differences in the mechanical behavior of the melt spun ribbons and nanoglass samples will be discussed in the present paper.

15 min. coffee break

MM 13.4 Mon 16:45 H52

Size effects in the deformation behavior of metallic nanoglass pillars — ●OMAR ADJAOUD and KARSTEN ALBE — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

Metallic nanoglasses (NGs) are amorphous materials with an inhomogeneous microstructure which consists of glassy grains connected by glass-glass interfaces. The metallic NGs can be produced by consolidating nanometer-sized glassy spheres which are prepared by inert-gas condensation. Glass-glass interfaces of metallic NGs are characterized by an excess free volume and a lack of short range order. This characteristics of the interfaces prevent the shear strain localization during the deformation of the metallic NGs, which leads to an enhanced plasticity in metallic NGs as compared to the bulk metallic glasses of the same chemical composition. In this contribution, we present the results of MD simulations on size effects in the deformation behavior of Cu₆₄Zr₃₆ and Pd₈₀Si₂₀ nanoglass pillars by varying systematically the diameter of the pillars from 4.5 nm to 54 nm. The results reveal that the pillars deform homogeneously due to their inhomogeneous microstructure. In contrast metallic glass pillars, with the same chemical composition, fail along a single shear band. Consequently, we assume that the deformation behavior of metallic glass pillars can be controlled by changing their microstructure rather than their size.

MM 13.5 Mon 17:00 H52

Analysis of the impact of nanocrystalline precipitates on the deformation behavior of a ZrCu based metallic glass — ●MARIUS GERLITZ¹, TOBIAS BRINK², MARTIN PETERLECHNER¹, HARALD RÖSNER¹, KARSTEN ALBE², and GERHARD WILDE¹ — ¹Institut für Materialphysik, WWU Münster, Germany — ²Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Due to the absence of dislocations in amorphous materials, plastic deformation of metallic glasses is carried by localized shear bands. In this work, the influence of nanocrystalline precipitates on the formation of shear bands is surveyed. To control the size and distribution of nanocrystallites within the amorphous phase, a crystallization study of the time and temperature dependence is carried out using differential scanning calorimetry (DSC). Structural analysis of partial crystallized samples is accomplished by transmission electron microscopy (TEM). Subsequently to the annealing procedure, the deformation of the material is enforced via cold rolling using a two-high rolling mill. By this means shear bands are induced inside the material. TEM analysis of the annealed and deformed metallic glass reveals the interaction between shear bands and nanocrystallites. Experimental results are compared to results of molecular dynamics simulations concerning different types of shear band particle interactions. The financial support of the DFG is gratefully acknowledged.

MM 13.6 Mon 17:15 H52

Shear band diffusion in cold rolled Pd₄₀Ni₄₀P₂₀ bulk metallic glass micro-alloyed with Co — ●MIKHAIL SELEZNEV^{1,2}, ISABELLE BINKOWSKI¹, SERGIY DIVINSKIY¹, and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Togliatty State University, Togliatty, Russia

Bulk metallic glasses (BMGs) appear to be promising materials due to a unique combination of glass-like elastic limit, hardness, corrosion resistance but without a ceramic-like brittleness. Although BMGs show some plasticity, their application is hindered due to deformation localization in shear bands (SBs). The shear banding mechanism seems to be the main reason for early failure in deformation and a key parameter that governs plasticity of BMGs.

Micro-alloying of the master alloy Pd₄₀Ni₄₀P₂₀ glass with Co (1 at.%) was found to increase the plasticity during compression by 13% [1]. This strong enhancement was accompanied by significant branching of SBs which could be due to a change in the work softening process and also by an increase of the free volume. To clarify a possible correlation between the micro alloying-induced plasticity increase and the SB structure changes, the atomic diffusivity was measured in deformed samples by the radiotracer technique and the results are discussed in relation to the Co-free PdNiP glass.

A financial support of DFG via SPP 1594 and DAAD together with the Ministry of Education and Science of the Russian Federation (project 3723) is acknowledged.

1. Nollmann N. et al. Scr. Mater. 111, 119 (2015)

MM 14: Transport II: Atomic and ionic transport

Time: Monday 15:45–17:30

Location: H53

MM 14.1 Mon 15:45 H53

Finding ultrafast diffusion in cold-rolled Nickel — ●SIMON TRUBEL¹, SERGIY DIVINSKI¹, MARTIN PETERLECHNER¹, CHRISTIAN SIMON¹, EHUD ALMOG², ERHARD SCHAFER³, and GERHARD WILDE¹ — ¹Institut für Materialphysik, WWU Münster — ²Dep. of Materials Science Engineering, Technion, Haifa — ³Physics of Nanostructured Materials, University of Vienna

Ultrafast diffusion rates have been found in a number of severely plastically deformed (SPD) materials. SPD processing produces an ultrafine grained microstructure while, at certain conditions, is able to modify grain boundaries into a specific (*non equilibrium*) state, at least a fraction of them. This fact was unambiguously shown for nickel of 99.6% purity deformed via ECAP or HPT [1]. At this point, an open question arises - does a critical deformation exist which would correspond to an appearance of such a characteristic state of grain boundaries?

Cold rolled Nickel of the same purity was investigated applying different deformation methods. Partial annealing of cold rolled nickel was found to open diffusion channels with characteristics alike to a

porosity network. The formation of these paths was investigated via x-ray diffraction and electron microscopy in combination with calorimetric analysis. Grain boundary self-diffusion was measured applying the ⁶³Ni radioisotope and precision mechanical sectioning. The results are discussed concerning the formation conditions of grain boundaries that would act as ultrafast diffusion paths.

[1] S. V. Divinski, et al. Acta Mater., 59, 1974 (2011).

MM 14.2 Mon 16:00 H53

Effect of precipitation on grain boundary diffusion in an Al-based alloy — ●BENGÜ TAS KAVAKBASI¹, VLADISLAV KULITCKII², SERGIY V DIVINSKI¹, and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48341 Münster, Germany — ²Belgorod State University, Belgorod, 308015, Russia

Precipitation phenomena affect the kinetics of diffusion in the surrounding matrix. The present study is focused on the effect of Al₃Sc precipitates on grain boundary diffusion in an Al-based AA5420 alloy (Al-4.6Mg-0.64Mn-0.2Sc-0.09Zr-0.2Ti-0.08Fe-0.02Si). Different states

were prepared by combination of ECAP processing and heat treatments and the radioisotope ^{57}Co was employed as a sensitive probe of a given grain boundary state. The results suggest that Co diffusion at room temperature is intimately coupled to the precipitation behavior of Al_3Sc at elevated temperatures. In fact, the Co diffusion coefficients are first decreasing with increasing precipitate size and approach a minimum at their average size of about 20 nm, which is probably related to maximal elastic stresses around the precipitates. As the precipitates grow further, the diffusion coefficients begin to increase due to a loss of coherence accompanied by a change in the chemical composition and a reduction of stresses around the precipitates.

Financial support of DFG via SPP1713 is gratefully acknowledged.

MM 14.3 Mon 16:15 H53

Hydrogen sorption kinetics of titanium hydride thin films — ●LUKAS MICHAŁEK, EFI HADJIXENOPHONTOS, and GUIDO SCHMITZ — University of Stuttgart, Institute for Materials Science, Heisenbergstrasse 3, 70569 Stuttgart, GERMANY

Titanium hydride has been studied a lot in the last few years because of its impressive hydrogenation kinetics. Transition metals are known to improve hydrogen (H) storage materials and act as catalysts in the diffusion process. Despite the low weight percentage of H it can take (4wt.%), it is a material in which H diffuses very easily and furthermore it's stable in air. In this work, we focus on the H-sorption behavior in thin films of thickness 50-400nm in different conditions. Pure α -Ti samples were deposited by ion beam sputtering on Si substrates. Hydrogenation was studied at different temperatures (RT-300°C) at 1-10 bars of H atmosphere for different duration of time (60-600min) in order to measure the kinetic barriers at the interfaces and diffusion coefficients. Hydrogen sorption was quantified by X-ray Diffraction, TEM was used for microstructural analyses and surface analysis was studied by SEM. A pure δ -TiH₂ peak appears in the XRD characterization for samples hydrogenated over 100min at 300°C and 10bars of H. Full dehydrogenation of this material is more challenging because of the stability of the hydride. Also the substrate choice appears to play an important role. Possible reversibility of δ -TiH₂ to α -Ti has been studied on magnesium oxide and aluminum oxide. The observed sorption behavior at these conditions will be the focus of this work.

15 min. coffee break

MM 14.4 Mon 16:45 H53

Descriptors of lithium-ionic conductivity from first-principles molecular dynamics — ●LEONID KAHLE¹, ARIS MARCOLONGO¹, NICOLA MARZARI¹, and BORIS KOZINSKY² — ¹Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — ²Robert Bosch LLC, Research and Technology Center, Cambridge, Massachusetts 02142, USA

We present a high-throughput study of lithium-ion conductivities obtained from extensive first-principles molecular dynamics simulations. Structures and trajectories are analyzed using methods and algorithms mutated from the field of computational geometry. First, we introduce a rigorous approach to discretize the volume of any arbitrary crystal

structure into physically meaningful interstitial sites. Then, we illustrate how to track atoms or ions of interest through the course of a simulation and how to detect jumps between interstitial sites with high spatial and temporal resolution. This approach allows us to correlate dynamical, structural and chemical properties of sites and materials with observables such as occupation densities and jump frequencies. We will conclude with the results obtained analyzing 3300 Born-Oppenheimer molecular dynamics simulations performed on 1200 Li-containing structures at varying temperatures, with the aim of identifying critical descriptors for Li-ion transport.

MM 14.5 Mon 17:00 H53

Transport of ions in a mixed Na^+/K^+ ion conducting glass - electrodiffusion profiles and electrochemical interphase formation — ●JOHANNES MARTIN¹, SARAH MEHRWALD¹, MARTIN SCHÄFER¹, THILO KRAMER², CHRISTIAN JOOSS², and KARL-MICHAEL WEITZEL¹ — ¹Fachbereich Chemie, Philipps-Universität Marburg — ²Institut für Materialphysik, Universität Göttingen

The competition of Na^+ ion versus K^+ ion transport in a mixed alkali borosilicate glass has been investigated by low energy bombardment induced ion transport employing Cs^+ ions as the foreign ion. Electrodiffusion causes the replacement of Na^+ and K^+ down to about 200 nm below the surface of the glass. Beyond this electrodiffusion front (in the direction of ion transport) K^+ ions accumulate to a density above the bulk concentration while Na^+ is further depleted towards the backward electrode. At the backward electrode only Na is electrodeposited since the electrical potential does not allow for K electrodeposition. A full simulation of the electrodiffusion profiles reveals the complete concentration dependence of the diffusion coefficients of the Na^+ and K^+ ions.

MM 14.6 Mon 17:15 H53

The mechanism of mixed ionic and electronic transport during electro-thermal poling — ●MARTIN SCHÄFER and KARL-MICHAEL WEITZEL — Fachbereich Chemie, Philipps-Universität Marburg

Electro-thermal poling is a technique that allows to investigate and manipulate physical properties of solid electrolytes, e.g. ion conducting glasses, in particular at the sample surface. During the poling experiment, the sample is placed between two ion blocking metal-electrodes and an electric field is applied at elevated temperatures. The charge carriers inside the sample move according to the field and give rise to an ion depletion zone below the anode. Usually, the buildup of the depletion zone is accompanied by the decay of the poling current and by the simultaneous expulsion of the field from the bulk of the sample such that eventually a strong field remains in the depletion zone solely. Here, a calculation based on a Monte-Carlo simulation is presented that describes the mechanism of electro-poling in samples with more than one mobile carrier species. The model explicitly includes the diffusion of two ion species and the electron mobility at electric field strengths beyond the breakdown field strength. The calculations show that for certain ion mobilities, the time evolution of the potential and the current decay occur on significantly different time scales. Diffusion profiles are calculated and compared to experiments from literature. Very good agreement is reached.

MM 15: Poster session I

Posters should be displayed by 4 pm. The MM poster prize will be awarded during the annual general assembly on Wednesday evening.

Posters submitted to: Integrated computational materials engineering for design of new materials, Methods in Computational Materials Modelling, Structural Materials, Frontiers of Electronic Structure Theory, Transport, Microstructure and Phase Transformations, Mechanical Properties, Liquid and Amorphous Metals

Time: Monday 18:00–20:00

Location: Poster B3

MM 15.1 Mon 18:00 Poster B3

Forces in the KKR method — ●ROMAN KOVÁČIK, RUDOLF ZELLER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

An accurate calculation of the ionic forces in the Korringa-Kohn-

Rostoker Green function (KKR-GF) method is crucial for its applicability to large scale material science simulations. In turn, the calculation of forces relies on an accurate evaluation of the electrostatic potential, especially in the interstitial regions where the inter-site terms exhibit very poor convergence with the angular momentum expansion. We explore and analyze an alternative method for the

numerical solution of Poisson's equation, based on a direct integration within space-filling Voronoi polyhedra [1]. An accurate and efficient isoparametric integration scheme without the use of shape functions is employed [2]. Furthermore, an alternative summation form is applied to the expressions in the Ewald procedure [3]. This approach is implemented and tested within the KKR-GF framework in the KKR $_{nano}$ computational code [4].

- [1] A. Alam *et al.*, Phys. Rev. B 84, 205106 (2011).
 [2] A. Alam *et al.*, Phys. Rev. B 84, 045105 (2011).
 [3] R. Zeller, J. Phys.: Condens. Matter 27, 306301 (2015).
 [4] A. Thiess *et al.*, Phys. Rev. B 85, 235103 (2012).

MM 15.2 Mon 18:00 Poster B3

Statics and dynamics of point defects in TiC — ●HOSSEIN EHTESHAMI¹, WEIWEI SUN², and PAVEL A. KORZHAVYI¹ — ¹Materials Technology, Department of Materials Science and Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — ²Materials Theory, Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

In this study, we present the results of a systematic ab initio study of point defects in titanium carbide. The electronic spectra and atomic structures for the metal and non-metal vacancies, interstitials, and antisite defects (including the split interstitial and split antisite conformations) are calculated within the generalized gradient approximation of density functional theory, using the projector augmented wave method as implemented in the Vienna Ab-initio Simulation Package VASP. In many cases the symmetric point defect configuration is found to be unstable against a symmetry-breaking distortion via the Jahn-Teller mechanism. An enhanced stability of titanium dumbbells is obtained for sub-stoichiometric TiC where the dumbbells form clusters with the carbon vacancies. Possible migration pathways for point defects and their clusters are explored in order to create a database of possible mechanisms of self-diffusion in TiC. The obtained information about the electronic of point defects, as well as about their formation and migration energies, can be useful in experimental (spectroscopic) and theoretical (atomistic modeling) studies of TiC and related materials.

MM 15.3 Mon 18:00 Poster B3

Analysis of electronic and structural properties of surfaces and interfaces involving LaAlO₃ and SrTiO₃ — ●IRINA PIYANZINA^{1,2}, THILO KOPP², and VOLKER EYERT³ — ¹Institute of Physics, Kazan Federal University, Kremlyovskaya St. 18, 420008 Kazan, Russia — ²EP VI and Center for Electronic Correlations and Magnetism, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany — ³Materials Design SARL, 18 rue de Saisset, 92120 Montrouge, France

Recently, it was established that a two-dimensional electron system can arise at the interface between the two oxide insulators LaAlO₃ (LAO) and SrTiO₃ (STO) [A. Ohtomo and H. Hwang, Nature **427**, 423 (2004); S. Thiel *et al.*, Science **313**, 1942 (2006)]. This paradigmatic example furthermore exhibits magnetism between the non-magnetic oxides. Despite the huge amount of both theoretical and experimental work a thorough understanding has yet to be achieved.

The aim of the present study is to investigate the electronic properties and structural distortions of surfaces and interfaces based on LAO and STO by means of density functional theory. We analyzed the structural deformations of the LaAlO₃ (001) slab induced by hydrogen adatoms and oxygen vacancies at its surface. Moreover, we investigated the influence of surface reconstruction on the density of states and determined the spatial dependence of the density of state at the Fermi level for bare LaAlO₃ surfaces and LaAlO₃/SrTiO₃ interfaces. In addition, the Al-atom displacements and distortions of the TiO₆-octahedra were estimated.

MM 15.4 Mon 18:00 Poster B3

Machine Learning of Structural and Electronic Properties of Semiconductors — BENEDIKT HOCK^{1,2}, UTE WERNER¹, KARSTEN HANNEWALD^{1,2}, LUCA GHIRINGHELLI², MATTHIAS SCHEFFLER², and ●CLAUDIA DRAXL^{1,2} — ¹Humboldt-Universität zu Berlin, Berlin, DE — ²Fritz-Haber-Institut der MPG, Berlin, DE

High-level solid-state computational methods enable very precise calculations of material properties such as lattice parameters and band structures. However, they usually also require a considerable computational effort. In order to circumvent such time-consuming calculations, recently machine learning techniques have emerged as an alternative predictive tool with potentially high accuracy. For example, Ghir-

inghelli *et al.* [*] could predict the crystal structure of binary octet semiconductors with the LASSO regression technique applied on an extended feature space. Using a similar methodology, we demonstrate that the lattice parameter can be learned from purely atomic and dimer data. Further, we explore the viability of learning ab initio band gaps from atomic and dimer data and/or low cost tight-binding calculations.

[*]: L.M. Ghiringhelli *et al.*, Phys. Rev. Lett. 114, 105503 (2015)

MM 15.5 Mon 18:00 Poster B3

Anharmonically stabilized temperature-dependent cluster-expansions applied to β -NiTi — ●SASCHA B. MAISEL, DOMINIQUE KORBMACHER, BLAZEJ GRABOWSKI, and JÖRG NEUGEBAUER — Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, 40239 Düsseldorf, Germany

The high temperature state β -NiTi is unstable with respect to transformation to a low-symmetry state at lower temperatures and to different phases at off-stoichiometric compositions. This poses several methodological challenges when developing effective models for the Ni-Ti system, which are integral in order to understand its intrinsic shape memory effect. Using recently improved methods for the temperature-dependent cluster-expansion (CE) approach, we derive and compare a hierarchy of descriptions of varying sophistication for the β -Ni-Ti high-temperature state. These descriptions are all based exclusively on ab-initio data or an ab-initio-based thermodynamic upscaling method known as the TU-TILD method [1], but yield surprisingly different results. This high sensitivity to the DFT input parameters is a consequence of the strong relaxations and dynamical instabilities that are ultimately responsible for the material's shape-memory properties. The various approaches are critically discussed regarding both their computational efficiency and their ability to reproduce CALPHAD free energies.

[1] A. I. Duff *et al.*: PRB **91**, 214311 (2015)

MM 15.6 Mon 18:00 Poster B3

Accelerating path integral molecular dynamics — ●VENKAT KAPIL¹ and MICHELE CERIOTTI² — ¹Laboratory of Computational Science and Modelling, Institute of Materials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — ²Laboratory of Computational Science and Modelling, Institute of Materials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

The cost of modelling quantum nature of light nuclei in an ab initio setup is still prohibitive, despite many recent developments that reduce the computational overhead. We illustrate how multiple time step integrators, used simultaneously with ring polymer contraction and appropriate thermostatting schemes, can reduce the overhead of modelling nuclear quantum effects, while describing inter-atomic forces at high levels of electronic structure theory, virtually to zero. This approach can be used together with other accelerated path integral techniques, such as generalized Langevin equation thermostats or high-order factorizations of the Boltzmann operator.

MM 15.7 Mon 18:00 Poster B3

Probing texture-induced abnormal grain growth in polycrystalline materials in 4D — ●MINGYAN WANG, JULES DAKE, ANTON MANIN, and CARL KRILL — Institute of Micro and Nanomaterials, Ulm University, Germany

Although abnormal grain growth (AGG) has been investigated in polycrystalline materials for more than 70 years, our understanding of the underlying mechanisms remains incomplete. Conventional studies based on micrographs cannot capture the real physical processes that take place in 3D. Instead, a non-destructive 3D characterization method is needed to probe these phenomena. Employing three-dimensional x-ray diffraction (3DXRD) microscopy, we were able to collect a sequence of microstructural snapshots, which could then be combined into a full 4D (3D+time) dataset. Analysis of particle trajectories show that a subpopulation of grains grows much faster than expected, indicating the occurrence of AGG. Comparing the microstructural evolution in our sample to a simulation of normal grain growth, we find large discrepancies in coarsening behavior. By extending a 3D phase field simulation to include texture-dependent grain boundary properties, we achieve much better agreement with the measured changes in grain size and morphology.

MM 15.8 Mon 18:00 Poster B3

Temperature dependent fracture of defected graphene sheets: a Molecular Dynamics study — ●SAMANEH NASIRI and MICHAEL

ZAISER — Institute of Materials Simulation, Friedrich-Alexander University Erlangen-Nürnberg, 90762 Fürth, Germany

Pristine graphene is known as the strongest material in terms of its in-plane tensile strength- a property which makes it a candidate for novel structural applications on the nano scale. However defects are unavoidable during the synthesis and fabrication of graphene-based devices. In this Paper we investigate the effect of defects on the temperature-dependent rupture strength of graphene sheets, for two different types of defects, namely randomly distributed point defects (vacancies) and single extended defects (cracks). We first study the effect of different vacancy concentrations and crack sizes on the fracture strength of graphene sheets at various temperatures and interpret our results with reference to continuum fracture mechanics concepts which we generalize to account for discreteness of the atomic and defect structure.

Keywords: Graphene, Vacancies, Cracks, Temperature, Molecular Dynamics, Fracture Mechanics.

MM 15.9 Mon 18:00 Poster B3

A Compressed Sensing Approach to Select Accurate Atom-Centered Basis Functions for Advanced Density Functional and Quantum Chemistry — •NIKLAS MENZEL¹, CHENCHEN WANG^{1,2}, LUCA GHIRINGHELLI¹, GITTA KUTYNIOK³, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin, DE — ²University of California, Santa Barbara, USA — ³Technische Universität, Berlin, DE

The choice of basis sets is one of the most important factors in quantum chemical calculations. Commonly used basis sets for advanced exchange-correlation functionals are not sufficiently accurate to represent Kohn-Sham Hamiltonian and its eigenfunctions. This leads to basis set extensions, such as the most famous correlation-consistent basis sets by Dunning. Due to computational costs, such basis sets have been so far used mainly for light atoms and their molecules. We have developed a basis-set selection approach that makes use of compressed sensing (CS), a recently developed signal processing technique, based on l1-norm regularization. As introductory example, we select via our CS-based approach Gaussian basis functions (GTO) from a large pool of various GTOs. The number of chosen GTOs can be tuned. We calculate the total energy for atoms from H to O, and then extend to molecules, e.g. H₂, and O₂. For H, He, and Li, our total-energy results are within 0.05 % compared with STO-6G energies. Starting from Be, CS selected basis set provide significantly better results than STO-6G, even when only 5 GTOs are considered. Our new approach enables us to determine accurate basis sets for heavier atoms and molecules.

MM 15.10 Mon 18:00 Poster B3

Rapid theory-guided prototyping of ductile Mg alloys — ZONGRUI PEI^{1,2}, •MARTIN FRIÁK^{3,1,2}, STEFANIE SANDLÖBES^{4,1}, BOB SVENDSEN^{1,2,5}, DIERK RAABE¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung, GmbH, Düsseldorf, Germany — ²Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — ³Institute of Physics of Materials, Brno, Czech Republic — ⁴Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, Aachen, Germany — ⁵Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen, Aachen, Germany

Magnesium alloys are promising structural materials with high specific strength. However, their broader use is limited by their low formability at ambient temperatures. It is known that Mg alloys containing small amounts of yttrium or rare-earth (RE) elements exhibit up to 5 times higher room temperature ductility but finding other solutes with the same effect is highly desirable. In order to identify a method allowing for a corresponding rapid alloy and solute assessment, we analyze relations between the I₁ stacking fault energies, which were shown to be related to the macroscopic ductility in Mg alloys (Acta Mater. 60 (2012) 3011), and the atomic volume *V* of pure solutes, their electronegativity ν and bulk modulus *B*. Comparing the impact of solutes with that of yttrium we propose a single numerical quantity (called yttrium similarity index, YSI) that is based on these interrelations. We evaluate YSI for 2850 Mg-ternaries and identify 133 promising solute pairs not including any RE elements (New J. Phys. 17 (2015) 093009).

MM 15.11 Mon 18:00 Poster B3

An *ab initio* high throughput approach to identify Mg-alloys with exceptionally high yield strength — ZONGRUI PEI^{1,2}, DUANCHENG MA¹, •MARTIN FRIÁK^{3,1,2}, BOB SVENDSEN^{1,2,4}, DIERK RAABE¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung, GmbH, Düsseldorf, Germany — ²Aachen Institute for Ad-

vanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — ³Institute of Physics of Materials, Brno, Czech Republic — ⁴Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen, Aachen, Germany

Using *ab initio* calculations and symmetrized plane waves, we analyze the basal-plane generalized stacking fault energies in pure Mg and Mg-Y alloys and show that the knowledge of energies of only five specific points is sufficient to accurately predict the core structures and Peierls stresses of (a)-type edge dislocations in these alloys. Our five-point approach substantially reduces the computational cost related to the Peierls-Nabarro (PN) model and allows for a high-throughput application of the PN model to study Peierls stress changes in Mg upon alloying. We employ our approach to study Mg binary alloys containing nine rare-earth (RE) and 11 other solutes. Based on the Peierls stresses of these 20 Mg alloys calculated from the Peierls-Nabarro model, the solutes are divided into three groups according to the dislocation core structure, the magnitude of Peierls stress, and their either strengthening or softening effect (Phys. Rev. B 92 (2015) 064107).

MM 15.12 Mon 18:00 Poster B3

Sulfation kinetics of high temperature corrosion in waste to energy plants — •DANIEL OTT¹, FERDINAND HAIDER¹, and RAGNAR WARNECKE² — ¹Univ. Augsburg, Inst. f. Physik, 86135 Augsburg — ²Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion leads especially in waste-to-energy-plants to massive problems. At prevalent temperatures around 500°C-600°C corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlorides.

This reaction requires an atmosphere containing SO₂, H₂O, O₂ and releases HCl/Cl₂. In this work we present results for the reaction kinetics, which depends on different parameters, like temperature, gas stream, gas components or (catalytic)additives. The conversion rate is strongly dependent on the transformation of SO₂ to SO₃, which is catalyzed by the presence of iron and iron oxides. In parallel to the study of the reaction rate it is possible to characterize the loss of metal simultaneously. Furthermore the behaviour of chlorine during the process of the corrosion was investigated. Investigations (theoretical and practical) of real superheater deposits were conducted for a better understanding of the predominant reactions and comparability of laboratory experiments. Principles of the prevalent conditions and reactions in waste-to-energy-plants, especially at the superheaters, are shown and experiments regarding the kinetics are presented.

Project supported by: BMBF - MatRessource, project: VOKos

MM 15.13 Mon 18:00 Poster B3

Deoxidation of stainless steels during vacuum brazing — •CORNELIA KUNZ¹, WOLFGANG MAUS-FRIEDRICHS¹, SIMON SCHÖLER^{2,3}, ULRICH HÖLLÄNDER^{2,3}, and KAI MÖHWALD^{2,3} — ¹Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Germany — ²Institut für Werkstoffkunde, Bereich Füge- und Oberflächentechnik (Fortis), Leibniz Universität Hannover, Germany — ³Institut für Werkstoffkunde, Leibniz Universität Hannover, Germany

Stainless steels are in widespread use due to their excellent mechanical and corrosion-proof properties. Corrosion resistance stems from native oxide layers formed on the surface of stainless steels, only a few nanometers thick and consisting of a mixture of chromium and iron oxides and hydroxides.

However, when choosing to join stainless steels by the means of vacuum brazing, the oxide layer prevents the wetting of the surface with braze, therefore inhibiting the joining process. Thus, deoxidation is a necessity. While procedural knowledge is abundant, fundamental understanding of thermophysical and chemical processes is lacking. Deoxidation is studied with two different stainless steels, AISI 304 and 446. Effect of heat treatment during vacuum brazing is recreated in laboratory scale by electron impact heating. Chemical analysis before and after heat treatment is carried out by XPS, AES and EDX/ WDX, optical and topographical properties are studied by CLSM. Bulk changes can be separated from surface changes due to different information depths of XPS/ AES and EDX/ WDX.

MM 15.14 Mon 18:00 Poster B3

Atomistic simulation of the early stages of precipitation in Al-Si-Mg alloys — •DANIELE GIOFRÈ and MICHELE CERIOTTI —

Laboratory of Computational Science and Modelling - EPFL, Lausanne, Switzerland

In the solid state the ternary phases exist mainly outside the fields of their primary crystallization. In the compositional range of 6XXX series aluminum alloys all phases, which form during the solidification, are of eutectic origin and are generally the result of non-equilibrium solidification (quenching mode). Furthermore, their properties are determined by the formation of coherent precipitates containing Mg, Al, Si.

In order to control the aging mode, namely the final result, an analysis of the stability and kinetics of these precipitates is of great importance in the Al-metallurgical industry. For these reasons it is particularly advantageous to have a mastery of the little-known early stages of precipitation. Therefore we want to study these small nuclei in order to investigate the aggregation of solute atoms, the critical sizes of nano-particles of the β'' phase, and their associated driving forces.

In the regime of this process, we have used a first-principles theory to conduct both the strength and stability study of the finite-size embedded precipitates nuclei of the β'' phase in the Al-bulk. We have carried out all that in order to compare the results with the simulation of formation energy, and to discover which is the morphology and stability of early precipitates and their thermodynamic driving force.

MM 15.15 Mon 18:00 Poster B3

Theoretical investigation of BiTeX (X=Cl,Br,I): Crystal structure and optical conductivity — ●RENÉ WIRNATA¹, SEBASTIAN SCHWALBE¹, GIULIO A.H. SCHOBER², JENS KORTUS¹, and RONALD STARKE¹ — ¹TU Freiberg, Institute for Theoretical Physics, Germany — ²University of Heidelberg, Institute for Theoretical Physics, Germany

Recently, the group of bismuth tellurohalides (BiTeX, X=Cl,Br,I) has been discovered to show a giant bulk Rashba splitting [1] that can be used e.g. in spintronics applications or magneto-optical devices [2,3]. Starting from X-ray data [4], we have constructed mono and double layer models of the experimental crystal systems. Using density functional theory, we discover a graphene/graphite-like band-crossing, which can also be observed in the low-frequency region of the optical response tensor. This may provide a new method for structural characterization by performing optical conductivity measurements.

Furthermore, this materials class shows a layered electron localization around the X and Te atoms, which manifests itself in the form of an increased conductivity in this plane.

- [1] Bahramy, M. S. et al., Phys. Rev. B, vol. 84, p. 041202
- [2] Lee, J. S. and Schober, G. A. H. et al., PRL, vol. 107, p. 117401
- [3] Demkó, L. and Schober, G. A. H. et al., PRL, vol. 109, p. 167401
- [4] Shevelkov, A. V. et al., J. Sol. St. Chem., vol. 114, pp. 379 - 384

MM 15.16 Mon 18:00 Poster B3

A fast Fermi orbital based self-interaction correction: Analytic 2nd order derivatives — ●CHARLOTTE VOGELBUSCH, LENZ FIEDLER, TORSTEN HAHN, and JENS KORTUS — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

One of the widely used electronic structure theories, density functional theory (DFT), is still limited due to systematic errors, e.g. the self-interaction error [1]. A new approach of a self-interaction correction (SIC) using Fermi orbitals has been initiated by Pederson, Ruzsinszky and Perdew [2].

The optimization of the Fermi orbital positions calculated with well established methods like the conjugate gradient results in high computational effort. In order to accelerate the slow convergence, some preconditioning for the numerical optimization of the SIC energy is needed. In this context the calculation of its derivatives is useful. The first order derivative of SIC energies has been investigated analytically by Pederson [3].

For preconditioning, the diagonal elements of the second order derivative have been analytically calculated. In the present work, this analytic approach has been benchmarked against numerical results for a set of small molecules.

- [1] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
- [2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
- [3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

MM 15.17 Mon 18:00 Poster B3

A fast Fermi orbital based self-interaction correction: A preconditioned Conjugate Gradient algorithm — ●LENZ FIEDLER, CHARLOTTE VOGELBUSCH, TORSTEN HAHN, and JENS KO-

RTUS — TU Freiberg, Institute for Theoretical Physics, Germany

In order to optimize methodical errors of density functional theory (DFT), a sufficient self-interaction correction (SIC) is needed. A possible approach is realized by the construction of localized orbitals such as Fermi orbitals, which can be obtained from Kohn-Sham orbitals. A full theoretical description of such a Fermi orbital based SIC is given by Pederson [1,2] drawing on previous results by Perdew and Zunger [3]. The implementation of this approach in a DFT code causes some numerical problems, due to the slow convergence in the optimization of the Fermi orbital positions.

Therefore we present an implementation of a conjugate gradient algorithm that is likely to improve the convergence of the calculation and therefore decreases the computational time. This is done by using a preconditioner which is composed of the diagonal elements of the Hessian of the energy function. These diagonal elements have been implemented both analytically and numerically. We show benchmarks against each other for a set of small molecules.

- [1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
- [2] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
- [3] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)

MM 15.18 Mon 18:00 Poster B3

Kondo effect in Dirac and Weyl semimetals — ●ANDREW MITCHELL and LARS FRITZ — Institute for Theoretical Physics, Utrecht University, 3584 CE Utrecht, The Netherlands

Magnetic impurities in three-dimensional Dirac and Weyl systems are shown to exhibit a fascinatingly diverse range of Kondo physics. When the Fermi level is precisely at the Dirac point, Dirac semimetals are in fact unlikely candidates for a Kondo effect due to the pseudogapped density of states. However, the influence of a nearby quantum critical point leads to the unconventional evolution of Kondo physics for even tiny deviations in the chemical potential.

Separating the degenerate Dirac nodes produces a Weyl phase: Time-reversal symmetry breaking precludes Kondo physics due to an effective impurity magnetic field, but different Kondo variants are accessible in time-reversal invariant Weyl systems. We study the distinctive spectroscopic signatures expected from scanning tunneling spectroscopy (STS), and also quasiparticle interference (QPI) where Kondo scattering is confined to surface Fermi arcs.

- [1] A. K. Mitchell and L. Fritz, Phys. Rev. B 92, 121109(R) (2015)

MM 15.19 Mon 18:00 Poster B3

Hydrogen sorption kinetics in magnesium and titanium hydride thin films — ●EFI HADJIXENOPHONTOS, LUKAS MICHALEK, and GUIDO SCHMITZ — University of Stuttgart, IMW, Heisenbergstrasse 3, 70569 Stuttgart Germany

Magnesium hydride is a model material which is intensively studied for hydrogen sorption in the last few years. Beside its favorable abundance, it is known for its high weight capacity of about 7 wt.% of hydrogen (H). It's a reversible storage system. However, it suffers from slow kinetics which makes it operational at only high temperatures. Research has shown that transition metals (TM) can improve this properties. In this work, we focus on the H-sorption behavior in thin films of thicknesses between 50-400nm in different conditions. The focus is to compare the kinetic properties and diffusion coefficients between TiH₂ and MgH₂ and multilayers thereof. Mg requires a thin Palladium (Pd) film on top for the hydrogenation to take place. Pure Mg/Pd and Ti metals were deposited by ion beam sputtering on Si/SiO₂ substrates. Hydrogenation of these layers followed at different temperatures (RT-300°C) and for different duration of times (10-600min) at 1-20 bars of H atmosphere. Full dehydrogenation of the samples has been tested and is shown to be more challenging for the TiH₂ because of its stability. Microstructure was studied by TEM. SEM was used for surface analysis. XRD is applied to quantify the hydrogen-sorption process and diffusion coefficients. Quantitative measurements and evaluation at different temperatures will be presented that allow determination of diffusivity and surface reaction coefficients.

MM 15.20 Mon 18:00 Poster B3

Ion-Beam Sputtered Thin Li_xSi Films and Atomic Transport — ●FLORIAN STRAUSS¹, HARALD SCHMIDT¹, and PAUL HEITJANS² — ¹TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — ²Leibniz Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, Deutschland

Thin films of lithium-silicon compounds as well as of pure silicon, both

in the amorphous and the crystalline state, are promising high capacity anode materials for future battery applications. An investigation of atomic and ionic transport processes in these materials is needed for an optimisation of charging/discharging properties and power densities. Li_xSi can either be deposited from a segmented target consisting of elemental Si and metallic Li by reactive co-sputtering as shown in [1] or directly from a bulk Li-Si alloy target. While no value for x below 1 is achievable for Li-Si alloys, segmented targets have been shown to produce films with a value of $0.03 < x < 0.6$. Experiments with SIMS, XPS and XRD were used to further characterise the sputtered layers. Measurements of transport parameters can be done by a neutron reflectometry based method, recently proposed by Hüger et al. [2].

[1] F. Strauß et al., RSC Adv. 5, 7192 (2014).

[2] E. Hüger et al., Nano Lett. 13, 1237 (2013).

MM 15.21 Mon 18:00 Poster B3

Identification of structural bottlenecks for sodium ion transport in solid state sodium ion conductors — ●KAUSTUBH BHAT, STEFAN BLÜGEL, and HANS LUSTFELD — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Sodium ion conductors offer significant advantages for applications in large scale-energy storage systems. It was observed that the ionic conductivity of NASICON [1] materials is correlated to certain areas that were proposed to be structural bottlenecks to sodium ion transport [2]. We use density functional theory along with the Nudged Elastic Band Method [3] to calculate the energy barrier for transport pathways in the NASICON material sodium scandium phosphate $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3$. We apply stress to the crystal to calculate the change of the energy barrier with changing strain [4]. Using a constrained gradient descent method, we quantify the effect of the following structural features on the energy barrier: (a) interatomic distances, (b) areas between neighboring atoms and (c) volumes around mobile ions. This enables us to identify all relevant structural bottlenecks. – We acknowledge fruitful discussions with our experimental colleagues F. Tietz and M. Guin toward this work.

[1] Hong H.Y.P., MRB 11, 173-182 (1976).

[2] Winaud J.M. et al. J.Mater. Sci. 25, 4008-4013 (1990).

[3] Henkelman G. et al. JCP 113, 9901-9904 (2000).

[4] Hirschfeld J.A. et al. PRB 84, 224308 (2011).

MM 15.22 Mon 18:00 Poster B3

Quantum Oscillation Signatures of Pressure-induced Topological Phase Transition in BiTeI — ●JOONBUM PARK^{1,2}, KYUNG-HWAN JIN³, GEUNSIK LEE⁴, YOUNG JUNG JO⁵, EUN SANG CHOI⁶, WOUN KANG⁷, ERIK KAMPERT⁸, JONG-SOO RHYEE⁹, SEUNG-HOON JHI¹⁰, and JUN SUNG KIM¹⁰ — ¹Max-Planck-Institute for Chemical Physics of Soilds, Dresden, Germany — ²Max Planck Center for Complex Phase Materials, Pohang, South Korea — ³University of Utah, Salt Lake City, Utah, USA — ⁴UNIST, Ulsan, South Korea — ⁵Kyungpuk University, Daegu, South Korea — ⁶National High Magnetic Field Laboratory, Tallahassee, Florida, USA — ⁷Ewha Womens' University, Seoul, South Korea — ⁸Dresden High Magnetic Field Laboratory, Dresden, Germany — ⁹Kyung-Hee University, Suwon, South Korea — ¹⁰POSTECH, Pohang, South Korea

We report the pressure-induced topological quantum phase transition of BiTeI single crystals using Shubnikov-de Haas oscillations of bulk Fermi surfaces. Above a critical pressure $P \sim 2\text{GPa}$, the Shubnikov-de Haas frequency for the inner Fermi surface increases unusually with pressure, and the Shubnikov-de Haas oscillations for the outer Fermi surface shows an abrupt phase shift. In comparison with band structure calculations, we find that these unusual behaviors originate from the Fermi surface shape change due to pressure-induced band inversion. These results clearly demonstrate that the topological quantum phase transition is intimately tied to the shape of bulk Fermi surfaces enclosing the time-reversal invariant momenta with band inversion.

MM 15.23 Mon 18:00 Poster B3

Atomic structure and dynamic viscosity of liquid GeTe — ●HANS WEBER^{1,2}, MATHIAS SCHUMACHER³, PÁL JÓVÁRI⁴, WERNER SKROTZKI², RICCARDO MAZZARELLO³, and IVAN KABAN¹ — ¹IFW Dresden, Institute for Complex Materials, PO Box 270116, 01171 Dresden, Germany — ²Technische Universität Dresden, Institut für Strukturphysik, 01062 Dresden, Germany — ³RWTH Aachen University, Institute for Theoretical Solid State Physics, 52056 Aachen, Germany — ⁴Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, PO Box 49, 1525 Budapest, Hungary

The atomic structure of GeTe liquid alloy is studied by X-ray diffraction and neutron diffraction in the temperature range from 750 to 850 °C. Its dynamic viscosity is measured from 1000 to 680 °C, which is 55 °C below the solidification point, using an oscillating-cup viscometer. The structural parameters of liquid GeTe show small changes and the dynamic viscosity behaves in accordance to the Arrhenius law. The experimental structural data are modeled with the reverse Monte-Carlo simulation technique. Ge atoms are found to be mainly coordinated by Te atoms and to a less extent by Ge atoms. The formation of a small number of Te-Te bonds is also probable. The results obtained are in agreement with ab-initio molecular dynamics simulations.

MM 15.24 Mon 18:00 Poster B3

Phase Transformation in Alloyed Nanowires — ●MANUEL ROUSSEL, MARTIN SCHELLENBERGER, TIM LEHMANN, and GUIDO SCHMITZ — Institute for Materials Science, Stuttgart, Germany

Since the discovery of giant magnetoresistance, for which Albert Fert and Peter Grünberg have been awarded the 2007 Nobel Prize, thin magnetic films have attracted much interest. More particularly, multi-layered nanowires consisting of magnetic and nonmagnetic layers (FeNi/Cu, Ni/Cu, Fe/Cr, Co/Cu...) have been proven to exhibit outstanding properties which have straightforward applications: M-RAM (magnetic random access memories), nano-sensors, data storage... Most of the time, the bottle neck for the usage of such nanostructures is that their synthesis is not reliable, especially when it comes to producing very small wires, in the range of a few tens of nanometers diameter. We are exploring alternative synthesis routes in order to find a new self-ordering way of producing multilayered or core-shell nanowires which would be only based on diffusion processes and phase separation. Simply put, we would like to create a plain alloyed nanowire and provoke the formation of layers just by a well-designed heat treatment. We will first present our approach to grow alloyed metallic nanowires of various compositions. In order to do so, we adopted a process based on electro-deposition in porous membranes. Later on we will focus on the influence of the nanowire geometry on phase transformation during annealing.

MM 15.25 Mon 18:00 Poster B3

Low-temperature heat capacity and magnetization of CoCr-FeNi and CoCrFeNiMn high-entropy alloys — ●JOSUA KOTTKE¹, MARTIN PETERLECHNER¹, MAYUR VAIDYA^{1,2}, BLAZEJ GRABOWSKI^{3,4}, FRITZ KOERMANN^{3,4}, JÖRG NEUGEBAUER³, SERGIY DIVINSKI¹, and GERHARD WILDE¹ — ¹Westfälische Wilhelms-Universität Münster, Germany — ²Indian Institute of Technology Madras, Chennai, India — ³Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — ⁴Materials Science and Engineering, TU Delft, Delft, Netherlands

High entropy alloys, i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as a potential structural material due to attractive mechanical and physical properties. We report on the first measurements of low-temperature heat capacity of four- (CoCr-FeNi) and five-component (CoCrFeNiMn) high-entropy alloys in the temperature interval from 1.9 to 400 K. The measurements were performed with and without application of a magnetic field (8T). Furthermore, room-temperature hysteresis loop and magnetization were measured in these alloys. The experimental data are compared with density-functional-theory-based calculations and a close agreement is seen. The deviations between the mean-field based theoretical results and direct experimental data are discussed in terms of probable ordering effects.

MM 15.26 Mon 18:00 Poster B3

Corrosion scale dynamics — ●MARKUS TAUTSCHNIG, NICHOLAS HARRISON, and MICHAEL FINNIS — Imperial College London

The presence of solid corrosion products, such as iron sulphides and iron carbonates, can lead to a significant reduction in the corrosion rate. Therefore, a fundamental understanding from the atomistic to the continuum level of their formation, stability and growth behaviour is vital for the oil and gas field equipment sustainability.

A "hexagonal slab" mesoscale growth model is being developed. This model has been created in order to predict the growth rate for scales with mesoscale morphology in various chemical environments. Assuming a dense and adherent scale, grain boundaries are considered as preferential pathways for the transport of charged point defects through the scale. The model includes the long range Coulomb interaction between the moving charged defect species. Migration-reaction-diffusion

is simulated for the model geometry. The equations for the mobile species are solved numerically with a novel C++ code. Time dependent concentration profiles throughout the grain boundaries can be calculated.

MM 15.27 Mon 18:00 Poster B3

Wurtzite to rocksalt phase transitions in binary compounds — •NING WANG, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

A pressure-induced wurtzite-to-rocksalt phase transition is observed in many binary compound semiconductors, such as CdSe, GaN and w-SiC. We analyzed this transition with the generalized solid-solid nudged elastic band method and determined the enthalpy landscape with first-principles calculations. Our results show that at both lower pressure and higher pressure, CdSe, GaN, and w-SiC prefer the tetragonal transition path to the hexagonal path. Furthermore, at lower pressure, the tetragonal-sliding and tetragonal-compression paths have almost the same transition barrier due to a similar intermediate tetragonal structure. At higher pressure, this metastable structure cannot be stabilized and the tetragonal-sliding path becomes energetically more favorable. We furthermore test the performance of two force fields for CdSe, and find that neither of them is able to describe the enthalpy landscape with good accuracy.

MM 15.28 Mon 18:00 Poster B3

Integration of a Fast-Scanning Calorimeter into a He-cryostat — •DANIEL GAERTNER, MARTIN PETERLECHNER, CHRISTIAN SIMON, and GERHARD WILDE — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

The Fast-Scanning Calorimeter (FSC), also known as Chipcalorimeter, is a power compensated and small scaled Differential-Scanning Calorimeter. Typically, sample up to several micrometers in diameter can be investigated with high heating rates exceeding 10000 K/s. Two FSC sensor chips are used simultaneously, one sensor is used as a reference and the other for the sample. Depending on the thermal bath temperature it is expected to achieve even higher cooling rates under high vacuum in a He-cryostat, the Physical-Properties-Measurement-System (PPMS, QD-LOT). Another advantage is a switchable magnetic field up to 9 Tesla. The technical approach of this custom build system will be presented including calibration procedures. The present approach allows in-situ quenching of metallic glasses, and measurements of the magnetic contribution to the specific heat of high-entropy alloys.

MM 15.29 Mon 18:00 Poster B3

Atomistic study of the growth of a B33 NiZr crystal from the melt: Observation of five- and tenfold twinning — •M. GUERDANE — Karlsruhe Institute of Technology (KIT), IAM-CMS, Karlsruhe

The crystallization of Ni₅₀Zr₅₀ from the melt is studied by means of molecular dynamics simulation. We consider pseudo-two-dimensional growth by setting up cylindrical crystalline NiZr seeds with a CrB-type structure (B33) and which can grow freely in all directions perpendicular to the cylinder axis. The crystallization is characterized by the formation of a high density of almost stress-free twins. The structure of the twins is reminiscent of that of FeB-type as predicted by Parthe earlier [1]. Moreover, fivefold and tenfold twinning is observed. The twins-formation mechanism is discussed and compared with that in pure materials as well as with the recently observed tenfold (quasicrystalline) twinned dendritic microstructure in the NiZr system [2].

1. E. Parthe, Acta Cryst. (1976). B32, 2813

2. W. Hornfeck et al., arXiv:1410.2952 [cond-mat.mtrl-sci].

MM 15.30 Mon 18:00 Poster B3

pressure induced phase transition in XeF₂ — •GANG WU¹, XI-AOLI HUANG², YANPING HUANG², XIN LI¹, FANGFEI LI¹, and TIAN CUI^{1,2} — ¹National Laboratory of Superhard Materials, Jilin University, Changchun 130012, P.R. China — ²College of Physics, Jilin University, Changchun 130012, P.R. China

It is well known that high pressure will bring materials some unique properties such as metallization or superconductivity. XeF₂ was reported to metalize under pressure. However, there is still controversy on its high pressure structure between the recent experimental and theoretical research. In this study, in-situ Synchrotron X-ray diffraction, Raman spectra and theoretical calculations are used to investigate the structure of XeF₂ up to 94GPa. The experimental and theoretic

cal Raman spectra results indicate that the ambient structure of XeF₂ (I4/mmm) transforms into a Immm structure at 26GPa, and then high pressure phase (space group Pnma) appears at 56GPa. In the XRD study, the rietveld refinement results show that the I4/mmm structure (a=3.8242Å, c=6.7882Å, Z=2, 7.5GPa) changes into Immm at 26GPa (a=3.3789Å, b=3.4056 Å, c=6.5883Å, Z=2), and stabilizes with the pnma structure at 60GPa (a=4.5275Å, b=4.5025Å, c=6.4703Å, Z=4), which is in accordance with our Raman study.

MM 15.31 Mon 18:00 Poster B3

On the influence of temperature and dopant concentration on Cu-Si phase formation — •HONEYEH MATBAECHI ETTEHAD^{1,3}, STEFAN E. SCHULZ^{1,2}, and ALEXANDER HEINRICH³ — ¹Technische Universität Chemnitz, Center for Microtechnologies, D-09107 Chemnitz, Germany — ²Fraunhofer Institute for Electronic Nano Systems (Fraunhofer ENAS), Technologie-Campus 3, D-09126 Chemnitz, Germany — ³Infinion Technologies AG, Wernerwerkstr. 2, D-93049 Regensburg, Germany

One of the reliability issues of semiconductor devices is the interaction between Copper (Cu) and Silicon (Si) while contacting the solder material with the side wall of the semiconductor die. Cu from the lead frame can diffuse into Si by diffusing through the solder material. So, this could lead to crack or failure of the device due to strain that result from volume increase. Nucleation and growth of Cu₆Si precipitates in Si has been studied by thermal treatment of copper layer in the range of 250-450°C on various commercially available silicon substrates, high-doped and low-doped. For all of the base materials the reaction between Cu and Si starts at lower temperatures in the range of 300-350°C, and leads to the formation of Cu₃Si. Number density and diameter of precipitates for different base materials and annealings were assessed experimentally and characterized by means of FIB, SEM and optical microscope. The influence of different base materials on number density of the CuSi precipitation was investigated. Significant differences in number density and size of precipitates are seen for various temperatures and dopant concentrations and will be discussed.

MM 15.32 Mon 18:00 Poster B3

Phase-Field Study of Anisotropic γ' -Coarsening Kinetics in Ni-Base Superalloys with Varying Re and Ru Contents — •LESLIE TAFADZWA MUSHONGERA, MICHEAL FLECK, JULIA KUNDIN, FRANK QUERFURTH, and HEIKE EMMERICH — Material- und Prozesssimulation Universität Bayreuth, Universität Bayreuth, Germany

The coarsening kinetics of γ' -precipitates in single crystalline Ni-based superalloys is studied using phase-field simulations. At first, we discuss interdiffusion-limited γ' -coarsening in technologically relevant superalloys with the explicit inclusion of up to nine chemical components. The simulations show that an additional influence from the coherency strain leads to a substantially faster coarsening-evolution compared to the predictions from the LSW-theory. Second, we perform a virtual experiment to determine the influence of varying rhenium (Re) and ruthenium (Ru) additions on the temporal evolution of the γ - γ' microstructure under thermo-mechanical loads. We observe that a change in the Re content strongly alters the coarsening kinetics. On the contrary, it is found that Ru variations have no significant effect on the coarsening kinetics.

MM 15.33 Mon 18:00 Poster B3

Microstructure development of aluminum based alloys in additive manufacturing revealed from differential fast scanning calorimetry and metallographic studies — •BIN YANG¹, OLAF KESSLER², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Rostock, Germany — ²Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Rostock, Germany

To obtain the desired additive manufacturing (AM) fabricated aluminum-based alloy parts, the rapid solidification processes need to be investigated in-situ. Based on the calorimetric method (differential fast scanning calorimetry) developed for the study of metal particles, the solidification process of aluminum-based alloy powder-particles, i.e. AlSi10Mg, was studied, for the very first time, under AM relevant heating and cooling rate conditions. A preliminary series of DFSC heating and cooling experiments was conducted, applying cooling rates as high as 80,000 K/s. The differential fast scanning calorimeter traces revealed that the material undergoes a two-stage melting and solidification processes depending on heating and cooling rates. In particular, the solidification structure of the real time quenched single droplet was observed and analyzed with focused ion

beam (FIB), scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). This research proposed a new approach to research the solidification structure of single aluminum-based alloys particles used in AM technologies with precisely controlled size and extreme cooling rate.

MM 15.34 Mon 18:00 Poster B3

Cluster dynamics modelling for the precipitation in Al-Cu — ●TOBIAS STEGMÜLLER and FERDINAND HAIDER — Univ. Augsburg, Inst. f. Physik, 86135 Augsburg

A key role in the production of modern metal alloys is to understand the precipitation processes occurring during thermal treatments, by which many material parameters like hardness or corrosion resistance can be controlled. A lot of these processes are qualitatively well understood controlled by empirical approaches. Nevertheless there is still a lack of knowledge in the quantitative understanding of the evolution of precipitates.

One approach for the simulation of such processes is the so-called cluster dynamics. In this approach the precipitate size distribution evolves with time. For that the precipitates are divided into classes, which are characterized only by the number of solute atoms n they contain. The temporal evolution is done by solving an initial value problem for the concentration c_n of precipitates belonging to class n .

Up to now the model has already several times been successfully applied to the formation of a single precipitate phase in binary alloys in literature. Our aim is to extend the model for an application to a system with multiple precipitate phases. For this purpose the Al-Cu system was chosen due to its well known precipitation sequence: the system decomposes via the formation of GP-Zones and different metastable phases. For the modelling a size distribution for each phase is needed and the distributions have to be linked to one another to gather the precursor-successor relationships between the phases.

MM 15.35 Mon 18:00 Poster B3

Microstructure Effects on Nanometric Cutting Behavior of Silicon — ●ALEXANDER STUKOWSKI¹ and SAURAV GOEL² — ¹Technische Universität Darmstadt — ²School of Mechanical and Aerospace Engineering, Queen's University, Belfast, UK

Silicon is being used extensively in both single crystal and polycrystalline form for a wide range of applications. To enable the production of ultra-thin wafers for future microelectronic applications, it is vital to fully understand the mechanical response of the material at small length scales.

We use direct molecular dynamics simulation to study the mechanisms of plasticity during cutting of monocrystalline and polycrystalline silicon. Our simulations are based on an improved long-range potential, providing a more accurate picture of the atomic-scale mechanisms of fracture, ductile plasticity, and structural changes in Si.

The simulation results show a unique phenomenon of brittle cracking inclined at an angle of 45° to 55° to the cut surface, leading to the formation of periodic arrays of nanogrooves in monocrystalline Si, which provides new insights into previously published experimental results. Furthermore, during cutting, silicon is found to undergo solid-state directional amorphisation without prior Si-I to Si-II phase transformation, which is in direct contrast to many previously published MD studies on this topic. Our simulations also predict that the propensity for amorphisation is significantly higher in single crystal silicon than in polysilicon, signifying that grain boundaries ease the material removal process.

MM 15.36 Mon 18:00 Poster B3

Push-Out Behavior of Tungsten Fiber-Reinforced Tungsten — ●BRUNO JASPER¹, STEPHAN SCHÖNEN², JAN W. COENEN¹, TILL HÖSCHEN³, JOHANN RIESCH³, RUDOLF NEU^{3,4}, and CHRISTIAN LINSMEIER¹ — ¹FZ Jülich GmbH, IEK4 - Plasmaphysik, Jülich, GER — ²FZ Jülich GmbH, ZEA1 - Engineering und Technologie, Jülich, GER — ³IPP, Garching, GER — ⁴TU München, Garching, GER

Tungsten (W) with its many beneficial properties, ranging from low hydrogen retention to low erosion yields during plasma exposure, is the candidate material for first-wall application in future fusion powerplants. The major drawback when working with W is its high ductile to brittle transition temperature. To circumvent this and to improve the overall mechanical properties, a tungsten fiber-reinforced tungsten (W_f/W) composite material is under development. W_f/W is composed of a drawn W wire, coated with an interface layer, and a W matrix. If

a crack is introduced into the material energy dissipation mechanisms are enabled by the interface. They lower the crack tip energy, leading to extrinsic toughening and therefore to a pseudo-ductile behavior of the material.

For better understanding and more insight into the underlying micro-mechanisms, push-out tests on single-fiber W_f/W samples were performed. This experimental work, that also covers the influence of sample geometry, sample preparation and test setup, is compared to results of dedicated finite element models.

MM 15.37 Mon 18:00 Poster B3

Mono-energetic Positron Source (MePS) — ●THU TRANG TRINH¹, OSCAR LIECKE¹, WOLFGANG ANWAND¹, ANDREAS WAGNER¹, and REINHARD KRAUSE-RHEBERG² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — ²Martin-Luther Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Positron annihilation lifetime spectroscopy serves as an excellent tool for studies of open-volume defects in solid materials such as vacancies, vacancy agglomerates, dislocations, pores and voids. The intense mono-energetic positron beamline (MePS) at the ELBE accelerator developed for positron lifetime and conventional Doppler Broadening experiments offers a non-destructive investigation method to study of porous media as well as thin films as a function of thickness.

MM 15.38 Mon 18:00 Poster B3

Friction under active control — ●VICTOR PFAHL¹, WALTER ARNOLD^{1,2}, and KONRAD SAMWER¹ — ¹Physikalisches Institut, Universität Göttingen — ²Department of Materials Science, Saarland University

Dissipation of mechanical and kinetic energy at a sliding contact – better known as friction – strongly depends on the topological structure and chemistry of the contact and on the dissipation mechanism of the underlying material. But instead of varying these internal mechanisms we are using external acoustic excitations – which is called sonolubricity – to control friction actively.

Friction is measured with the lateral force microscopy (LFM) mode of an atomic force acoustic microscope (AFAM) with the simultaneous excitation of the contact resonance frequency of the AFAM cantilever. The cantilever is moving periodically resulting in a reduced average contact force and therefore the friction coefficient is reduced as well.

We investigated the reduction of friction of Si, PdCuSi, and LaSrMnO as a function of amplitude of the cantilever at different temperatures. We report a reduction of friction up to 100% on every sample. Due to a metal-insulator transition near 350K especially temperature dependent measurements on LaSrMnO are interesting. A different reduction – amplitude relation is found in the metallic phase in comparison to the insulating phase.

We thank the German Science Foundation for funding within the SFB CRC 1073, project A1.

MM 15.39 Mon 18:00 Poster B3

Influence of thermal and mechanical pre-treatment on the properties of bulk metallic glasses — ●NIKLAS OLSCHESKI¹, MORITZ STOLPE², CHRISTIAN SIMON¹, HARALD RÖSNER¹, RALF BUSCH², and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Germany — ²Chair for Metallic Materials, Department of Materials Science, Saarland University, Germany

Metallic glasses provide many advantageous properties such as high elasticity, wear resistance and yield strength. Despite these features and the possible merits for the use of metallic glasses in applications, the evolution of the microstructure in glasses upon external influences such as mechanical stress or temperature is still not fully understood. An example is the formation of so called shear bands, which evolve in glasses after a certain degree of deformation: the microscopic origin of such unit shear events is still unresolved.

The presented work focuses on the impact of mechanical pre-deformation and thermal treatment by calorimetry at different rates on the state of a bulk metallic glass. In particular the dependence of the materials properties on different strain rates during linear and cyclic deformation as well as the behavior of the glass-transition for various heating rates was investigated. The results of these investigations lead to an improvement in understanding; that is, how the history of a glass, whether mechanical or thermal, is linked to its macroscopic properties.

MM 16: Invited talk Derlet

Time: Tuesday 9:30–10:00

Location: H38

Invited Talk

MM 16.1 Tue 9:30 H38

Critical stresses in intermittent plasticity and the transition to macroscopic yield — ●PETER DERLET¹ and ROBERT MAASS² —¹Condensed Matter Theory Group, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — ²Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, 1304 West Green Street, Urbana, Illinois 61801, USA

A dislocated crystal will locally undergo discrete plastic deformation at virtually any applied stress. High resolution extensometry on bulk crystals or small scale deformation experiments display such discrete plasticity in stress-strain data. This talk focuses on the statistics of such plastic events in the regime prior to macroscopic yield. Extreme

value theory is applied to the critical stresses at which discrete intermittent plasticity occurs. It is found that when the same deformation is repeated many times in both experiments and dislocation dynamics simulations with strongly varying microstructures, the average of the critical stress and the Weibull fluctuations around it, is related to the deforming crystal volume via a truncated power-law. It's applicability across a rich data set suggests that a quite general phenomenon is at play. The identified truncated power-law is found to uniquely define an underlying master distribution of critical stresses present in the deforming crystal, and also the density of discrete plastic events available to the system. It therefore provides a procedure to experimentally characterize a material's microstructure both prior to loading and in the microplastic regime to yield.

MM 17: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science I

Time: Tuesday 10:15–11:45

Location: H38

MM 17.1 Tue 10:15 H38

Advanced AFM based electrical and mechanical characterization of nanostructured materials under controlled environment — ●CHRISTIAN TEICHERT, MARKUS KRATZER, IGOR BEINIK, CHRISTIAN GANSER, and FRANZ J SCHMIED — Institute of Physics, Montanuniversität Leoben, Austria

Besides morphological characterization, atomic-force microscopy (AFM) based techniques can successfully be employed to study physical properties on the nanometer scale under controlled environmental conditions. Here, we will in particular focus on the measurement of electrical and optoelectronic properties of semiconductor nanostructures under simultaneous irradiation by light via photoconductive AFM and photo-assisted Kelvin Probe Force Microscopy [1-2]. With respect to mechanical characterization, AFM based nanoindentation experiments on cellulose films and fibers under controlled humidity will be presented [3-4]. Finally, procedures are introduced where the AFM is just used to apply and measure specific forces among nanostructures [5].

[1] M. Kratzer, et al., Phys. Rev. B 86 (2012) 245320. [2] I. Beinik, et al., Beilstein J. Nanotechnol. 4 (2013) 208. [3] C. Ganser, et al., Holzforschung 68 (2014) 53. [4] C. Ganser, et al., Bioinspired, Biomimetic and Nanobiomaterials 3 (2014) 131. [5] F.J. Schmied, et al., Sci. Rep. 3 (2013) 2432.

Topical Talk

MM 17.2 Tue 10:45 H38

Forces at the nanoscale: Sliding nanoparticles and pushing molecules — ●ANDRE SCHIRMEISEN — Justus-Liebig University Giessen, Giessen, Germany

The atomic force microscope (AFM) is an indispensable tool for surface characterization in material science down to atomic scales. While most force microscopy applications are related to surface structure characterization, recent progress has been reported in the field of AFM-based surface object manipulation. Minute forces can not only be detected by the cantilever-based sensors, but exerted in a controlled way. An example is the simultaneous manipulation and detection of lateral forces during nanoparticle sliding, relevant for our understanding of microscopic friction mechanisms. In particular the contact area dependence of friction for atomically defined interfaces was found to

obey a sub-linear scaling [1], contradicting the widely accepted linear Amontons law. In the extremely sensitive non-contact AFM mode, the tip-induced motion of individual atoms and molecules is possible. In the case of the perylene derivative PTCDA on Ag, the force needed to push the molecule by one atomic lattice site was measured [2], which is directly linked surface diffusion energy barriers. This progress opens the path to study material properties at nanoscale by controlled AFM manipulation techniques.

[1] D. Dietzel et al., Physical Review Letters 111 (2013) 235502.

[2] G. Langewisch et al., Physical Review Letters 110 (2013) 036101.

MM 17.3 Tue 11:15 H38

Controlled scanning probe manipulation and lithography: What can be learned about mesoscale friction and abrasive wear? — ●ENRICO GNECCO^{1,2}, PATRICIA PEDRAZ², and REINHOLD WANNEMACHER² — ¹Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Germany — ²IMDEA Nanociencia, Madrid, Spain

Atomic force microscopy is an invaluable technique to investigate friction mechanisms on the nano- and mesoscale. We will first focus on nanomanipulation experiments and discuss how the trajectories of nanoparticles on solid substrates are related to the scan path followed by the AFM probe and the friction between particles and substrate. Irregularly shaped Sb islands and wavy glass surfaces are chosen as examples. The discussion will be extended to the formation of wear patterns on compliant surfaces also in relation to the AFM scan path. Solvent enriched polymers at room temperature are an optimum benchmark for this kind of experiments. In this case the dependence of wear patterns on the normal force and scanning velocity is easily explained by an extension of the well-established Prandtl-Tomlinson model for atomic-scale friction. In particular we observe a phase transition between wearless sliding and rippling of the substrate surface, which is reminiscent of the stick-slip/continuous sliding transition on the atomic scale. The wearless regime can also be entered by mechanical excitation of the contact resonance during the sliding.

15 min. coffee break

MM 18: Topical session: Integrated computational materials engineering for design of new materials IV

Time: Tuesday 10:15–11:45

Location: H39

Topical Talk

MM 18.1 Tue 10:15 H39

Robust crystal-structure prediction with structure maps — ●THOMAS HAMMERSCHMIDT — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges in materials design. The most common strategies are (i) the search for the energetically most favourable crystal structure by explicit atomistic calculations and (ii)

the identification of descriptors that allow extrapolations from known materials to unknown compounds. A promising approach of the second kind are structure maps that chart the bonding chemistry of known compounds. I will discuss two structure maps and motivate their descriptors that are based on physically intuitive functions of the number of valence electrons, the atomic volume and the electro-negativity. The first example, a structure map for complex intermetallic phases, is set up by electronic-structure considerations. This two-dimensional map correctly predicts the crystal structure of precipitates in multi-component Ni-base and Co-base superalloys. The second example is a three-dimensional structure map derived by a systematic cluster analysis of experimentally observed compounds of sp-block elements and transition metals. This map reaches a predictive power that is close to standard density-functional theory calculations. The identified descriptors remain valid for off-stoichiometric compounds and separate binary and ternary crystal-structure prototypes.

MM 18.2 Tue 10:45 H39

Better (random) walking through chemistry: how not to get lost in vast configurational spaces — ●CHIARA PANOSSETTI¹, KONSTANTIN KRAUTGASSER¹, DENNIS PALAGIN², KARSTEN REUTER¹, and REINHARD MAURER³ — ¹Technische Universität München — ²University of Oxford — ³Yale University

Ab initio structure prediction can systematically aid the computational discovery and rational design of new materials, as well as providing interpretative insights when atomistic details are difficult to resolve experimentally. However, global geometry optimization –the method of choice for finding chemically relevant (meta-)stable structures– is rarely applied to large-scale systems. The main challenge lies in the necessity of efficient ways to traverse configurational spaces in which the number of minima explodes with system size. We recently proposed an approach to global screening in chemically meaningful subspaces [1]. Following the *fil rouge* of the exploitation of chemically motivated trial moves, we now extend it to the study of organic molecules on surfaces –by suitably imposing partial constraints– and to complex interfaces with variable or unknown stoichiometry –by applying strategies to alleviate the strain of newly generated structures upon grand-canonical particle insertion. A selection of prototypical results will be presented (a retinoic acid analogue on Au(111) and metal-silicon clusters growth) to illustrate how all relevant portions of chemical space can be accessed with this approach, whereas “conventional” sampling often even struggles to produce sensible structures besides the starting geometry at all. [1] Nano Lett., doi: 10.1021/acs.nanolett.5b03388 (2015)

MM 18.3 Tue 11:00 H39

Chemically-motivated coordinates and their potential role

in efficient materials structure search — ●KONSTANTIN KRAUTGASSER¹, CHIARA PANOSSETTI¹, DENNIS PALAGIN², KARSTEN REUTER¹, and REINHARD MAURER³ — ¹Technische Universität München — ²University of Oxford — ³Yale University

Finding energetically favorable, chemically relevant structures is a main challenge for computational materials discovery. Especially for reactions in heterogeneous catalysis and the design of hybrid inorganic-organic interfaces we generally encounter a structural complexity that cannot be treated by a manual search of minimum energy structures. We propose automatically created delocalized internal coordinates (DICs) that adapt to the local chemistry as a key tool to enable more efficient global structure screening. DICs can be straightforwardly constructed for gas-phase or adsorbed systems, molecular aggregates, crystals and complex interfaces. The ability to enforce arbitrary constraints facilitates the search in chemically-motivated subspaces. We present the construction procedure and shape of DIC displacements for a representative gas-phase system, an organic adsorbate, and a dense molecular overlayer. We implemented this in a Python package (*winak*) that can be interfaced with a multitude of electronic structure and molecular mechanics modelling tools. The modular framework of the package enables direct community contribution and connection of these coordinates with a number of different global optimization procedures.

MM 18.4 Tue 11:15 H39

Tight-binding parameterizations across the periodic table — ●JAN JENKE¹, ALVIN LADINES¹, THOMAS HAMMERSCHMIDT¹, DAVID G. PETTIFOR², and RALF DRAUTZ¹ — ¹ICAMS, Ruhr-Universität Bochum, Germany — ²Materials Modelling Laboratory, Department of Materials, University of Oxford, UK

Tight-binding (TB) parameters may be obtained from density functional theory (DFT) by projecting the DFT wave functions on the TB minimal basis. We create a comprehensive database of TB parameters for all dimers of sp- and sd-valent atoms using the Harris-Foulkes wave function as reference. We demonstrate that the Hamiltonian matrix elements of the intrinsically non-orthogonal and the Loewdin-transformed orthogonal TB model, as well as the overlap matrix elements, can be satisfactorily fitted using a single functional form. This enables us to compute the bond energy, promotion energy and repulsive energy within the TB bond model and to carry out a systematic analysis of hybridization and screening effects. We extract trends of the TB parameters across the periodic table and verify the quality of the parameterizations for bulk structures.

15 min. coffee break

MM 19: Mechanical Properties I

Time: Tuesday 10:15–11:45

Location: H52

MM 19.1 Tue 10:15 H52

FUNDAMENTAL NANOMECHANIC INVESTIGATIONS USING COMBINATORIAL DEPOSITION TECHNIQUES — ●RACHEL SCHOEPPNER, LASZLO PETHO, and JOHANN MICHLER — Empa, Materials Science and Technology, Thun, Switzerland

We’ve designed a unique deposition system combining magnetron sputtering, e-beam evaporation, nanoparticle deposition and atomic layer deposition (ALD). An integrated shutter controller allows for creating thickness gradients of two or three different materials, which can then be annealed to create a combinatorial materials library with compositional gradients over almost the complete spectrum. Initial studies of the system capability have focused on proof-of-concept trilayer systems consisting of Al₂O₃ and TiO₂ ALD layers sandwiched between thicker Cu layers deposited by sputtering. Physical and mechanical characterisation of these trilayers, including micropillar compression, has demonstrated good interfacial adhesion and that even just a single ALD layer, only nanometers thick, can provide significant hardening to Cu thin films. Combinatorial libraries of ternary AlCuAu and AuAgPt alloy systems have been used in an adhesion study to examine the effect of composition on interfacial adhesion, between the film and a 500 nm thick layer of Al₂O₃ deposited using ALD. Finally, Cu films were reinforced via co-deposition of W nanoparticles. The microstructure, particle size and density were characterized using transmission electron microscopy and initial nanoindentation investigations were conducted

to determine how nanoparticle inclusion affects the hardness and modulus of the films.

MM 19.2 Tue 10:30 H52

Flaw sensitivity of nanowires — ●CHRISTIAN BRANDL — Institute for Applied Materials, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

With decreasing dimensions of the metals, the strength is increasing with decreasing dimensions can approach the theoretical strength limit - down to a regime, where the strength is theoretically predicted to be flaw insensitive.

Using atomic simulation, we investigate the effect of predefined flaws, i.e. notches, in intrinsic brittle Si nanowires and intrinsic ductile Au nanowires. The flaw size and wire diameter dependent strength and ductility in the molecular dynamics (MD) simulations show the existence of the flaw insensitive size regime. The defect evolution, flow stresses and the strain hardening in the MD simulations of Au nanowires is compared to experimental studies, where gold nanowires were structured by He-ion beams with sub-50 nm diameter well-defined holes. The experimental microstructure after deformation - as seen by (high-resolution) transmission electron microscopy - suggests the formation of a nano-grained substructure at the failure location, which is also consistently observed in our MD simulation.

The striking similarities between MD simulations and the experi-

mental data are critically discussed and explained by strain hardening in a strength regime of theoretical shear strength in Au. More generally, the implications of strain rate dependence and temperature dependence of the flow stresses are discussed for nanowires in the size regime of flaw insensitivity.

MM 19.3 Tue 10:45 H52

Metamaterials using buckling instabilities for reusable energy absorbers — •TOBIAS FRENZEL¹, CLAUDIO FINDEISEN^{2,3}, MUAMER KADIC¹, PETER GUMBSCH^{2,3,4}, and MARTIN WEGENER^{1,4} — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — ²Institute for Applied Materials, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — ³Fraunhofer Institute for Mechanics of Materials IWM, 79108 Freiburg, Germany — ⁴Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Commonly, structures and materials for mechanical energy absorption exploit either viscoelasticity or plasticity. While viscoelasticity leads to a reusable, yet time-dependent behavior, plasticity is not influenced by the timescale, yet the structural deformation is irreversible. In this work, we introduce a new class of artificial material, which exploits elastic buckling in a uniaxial micro-lattice as a mechanism for energy absorption. Most importantly the energy is not dissipated by local effects, e.g., within one unit cell, but by the coupling of N effectively nonlinear springs in series. By tailoring the buckling elements, either a hysteretic, yet repeatable, or a multi-stable behavior enabling for programmability can be achieved. Furthermore, the shape of the stress-strain curves can be tailored, which allows for control over peak forces. Experiments performed on polymer micro-structures made by direct laser writing scaled to aluminum show specific energy absorption comparable to state-of-the-art aluminum-foams.

MM 19.4 Tue 11:00 H52

Scaling laws of nanoporous gold under uniaxial compression: Effects of structural disorder on the solid fraction, elastic Poisson's ratio, Young's modulus and yield strength — •BENEDIKT ROSCHNING¹ and NORBERT HUBER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology — ²Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Recent investigations on the mechanical behavior of nanoporous gold [1,2,3] led to inconsistencies to previous results (summarized in [4]) indicating that the material's coupling behavior between the solid phase and the macroscopic mechanical response is still not fully clarified. We

investigated the relationship between the structural disorder and the macroscopic mechanical behavior of nanoporous gold under uniaxial compression, using the finite element method. Scaling equations for the elastic Poisson's ratio, the Young's modulus and the yield strength were determined as functions of the structural disorder and the solid fraction. The model was applied to identify the elastic-plastic material behavior of the solid gold phase. Based on this approach, a systematic study of the size effect on the yield strength was performed and the results were compared to experimental data provided in literature. An excellent agreement with recently published results for samples of nanoporous gold with varying ligament size was found. [1] Huber, N., et al. 2014. *Acta Materialia* 67, 252-265. [2] Jin, H.-J., et al., 2009. *Acta Materialia* 57, 2665-2672. [3] Wang, K., et al., 2015. *NPG Asia Mater* 7, e187. [4] Weissmüller J., et al., 2009. *MRS Bulletin* 34, 577-586.

MM 19.5 Tue 11:15 H52

Stacking fault energetics of α - and γ -cerium investigated with ab initio calculations — •ANDREAS ÖSTLIN¹, IGOR DI MARCO², INKA LOCHT², JASON LASHLEY^{2,3}, and LEVENTE VITOS^{1,2,4} — ¹Applied Materials Physics, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — ²Department of Physics and Materials Science, Uppsala University, P.O. Box 516, SE-75120 Uppsala, Sweden — ³Los Alamos National Laboratory, P.O. Box 1663 Bikini Atoll Road, Los Alamos, New Mexico, USA — ⁴Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

At ambient pressure the element cerium shows a metastable double hexagonal close-packed β -phase that is positioned between two cubic phases, γ and α . We have computed stacking fault formation energies of the cubic phases of cerium using an axial interaction model. Total energies were calculated by density functional theory (DFT) and by dynamical mean field theory (DMFT) merged with density functional theory (DMFT+DFT). It is found that there is a large difference in the stacking fault energies between the α and γ -phase. The β -phase energy is nearly degenerate with the γ -phase, consistent with previous third law calorimetry results, and dislocation dynamics explain the pressure and temperature hysteretic effects. The β -phase can be seen as a dislocation reservoir that appears to be necessary to accommodate the large strains generated during the α - γ transition.

15 min. coffee break

MM 20: Topical session: Caloric Effects in ferroic materials I - Magnetocalorics

Time: Tuesday 10:15–11:45

Location: H53

MM 20.1 Tue 10:15 H53

The coupling of electronic, magnetic and lattice degrees of freedom in the magnetocaloric system La-Fe-Si — •MARKUS E. GRUNER^{1,2}, WERNER KEUNE¹, BEATRIZ ROLDAN CUENYA³, CLAUDIA WEIS¹, JOACHIM LANDERS¹, SOMA SALAMON¹, BENEDIKT EGGERT¹, SERGEY I. MAKAROV¹, DAVID KLAR¹, MICHAEL Y. HU⁴, ERCAN E. ALP⁴, JIYONG ZHAO⁴, MARIA KRAUTZ⁵, OLIVER GUTFLEISCH⁶, and HEIKO WENDE¹ — ¹Universität Duisburg-Essen — ²Forschungs-Neutronenquelle FRM II, Garching — ³Ruhr-Universität Bochum — ⁴Argonne National Laboratory — ⁵IFW Dresden — ⁶TU Darmstadt

LaFe_{13-x}Si_x counts in its hydrogenated form as one of the most promising magnetocaloric materials for application. By combination of nuclear resonant inelastic X-ray scattering and first-principles calculations in the framework of density functional theory, we could recently demonstrate an unexpected phonon softening at the magnetic phase transition of pure La-Fe-Si, which contributes cooperatively with the magnetic degrees of freedom to the large magnetocaloric effect. The softening is traced back to adiabatic electron phonon coupling which originates from specific changes in the electronic density of states at the Fermi Level due to the itinerant electron metamagnetism of Fe [1]. Within this contribution we will review the signatures of itinerant electron metamagnetism and its implication for the magnetoelastic coupling in pure, Mn-doped and hydrogenated La-Fe-Si. Funding by the DFG (SPP1599, TRR80) is gratefully acknowledged.

[1] M. E. Gruner, W. Keune, B. Roldan Cuenya *et al.*, *Phys. Rev. Lett.*

114, 057202 (2015)

MM 20.2 Tue 10:45 H53

Element-resolved vibrational dynamics and thermodynamics of magnetocaloric FeRh compound — •WERNER KEUNE¹, MARKUS E. GRUNER¹, JOACHIM LANDERS¹, SOMA SALAMON¹, FRANZISKA SCHEIBEL¹, DETLEF SPODDIG¹, BEATRIZ ROLDAN CUENYA², OLIVER GUTFLEISCH³, MICHAEL Y. HU⁴, JIYONG ZHAO⁴, THOMAS TOELLNER⁴, ERCAN E. ALP⁴, and HEIKO WENDE¹ — ¹Universität Duisburg-Essen, Germany — ²Ruhr-Universität Bochum, Germany — ³TU Darmstadt, Germany — ⁴Argonne National Laboratory, USA

Employing both ⁵⁷Fe nuclear resonant inelastic X-ray scattering and first principles calculations (DFT), similar to ref. [1], we determined the Fe-projected phonon DOS of the B2-ordered magnetocaloric FeRh compound at temperatures below and above the first-order magnetostructural phase transition from the antiferromagnetic (AFM) to the ferromagnetic (FM) state. Two experimental ⁵⁷FeRh(001) thin-film samples on MgO(001) with different stoichiometries (AFM and FM, respectively) were studied. Distinct differences between the phonon DOS of the AFM and FM states were found. However, this leads only to very small differences in the T-dependences of the Fe-projected vibrational (lattice) specific heat $C(T)$ and the vibrational entropy $S(T)$, respectively, for the two magnetic states. The experimental Debye-Waller factor indicates that the lattice of the AFM state is softer than in the FM state.

[1] M. E. Gruner et al., Phys. Rev. Lett. 114, 057202 (2015).

MM 20.3 Tue 11:00 H53

Understanding the magnetostructural transitions of first-order materials — ●TINO GOTTSCHALL, DIMITRI BENKE, KONSTANTIN SKOKOV, MAXIMILIAN FRIES, ILIYA RADULOV, and OLIVER GUTFLEISCH — TU Darmstadt, Material Science, Darmstadt, Germany

The large magnetocaloric effect in the most promising first-order materials like La-Fe-Si [1], Fe₂P type materials [2] or Heusler alloys [3] originates in the strong change of the magnetization with temperature being associated with a structural transformation. All these materials have one thing in common. The so-called magnetostructural transition goes hand in hand with a large volume change or at least a large change of the *c* to *a* ratio of the crystal structure.

In this work we present magnetic measurements of micrometer sized single particles of the three mentioned materials and compare them with the transformation characteristics of the corresponding bulk properties. It turns out that a very different behavior is observed depending on the size of the magnetocaloric sample. This result is of great importance for the application of magnetic refrigeration, especially for the design of powder bed heat exchangers.

This work was supported by DFG (Grant No. SPP1599)

[1] I.A. Radulov, K.P. Skokov, D.Yu. Karpenkov, T. Gottschall, O. Gutfleisch, J. Mag. Mag. Mater. 396 (2015) 228 [2] F. Guillou, H. Yibole, G. Porcari, L. Zhang, N.H. van Dijk, E. Brück, J. Appl. Phys. 116 (2014) 063903 [3] T. Gottschall, K.P. Skokov, B. Frincu, O. Gutfleisch, Appl. Phys. Lett. 106 (2015) 021901

MM 20.4 Tue 11:15 H53

MM 21: Microstructure and Phase Transformations I

Time: Tuesday 11:45–13:15

Location: H38

MM 21.1 Tue 11:45 H38

Undercooling behavior of the nucleation of liquid-liquid phase — ●CHRISTIAN SIMON¹, YIKUN ZHANG², and GERHARD WILDE¹ — ¹Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48155 Münster — ²State Key Laboratory of Advanced Special Steels, Shanghai University, Shanghai, 200072, China

A wetting transition from partial wetting to complete wetting is possible in alloys with a liquid miscibility gap. At a temperature T_p below the critical temperature T_c , the alloy separates in a two-phase liquid system which plays an essential role in the microstructure formation of monotectic alloys. A thermal cycling in the liquid state allows observing the mixing and the demixing transition. This allows a monitoring of the statistical behavior of the phase transition temperatures over a large number of cycles. We present data of the copper-cobalt and the copper-iron system obtained by classical DTA experiments. The copper-cobalt and the copper-iron system have a metastable miscibility gap. The interest is here in the observation of the undercooling behavior. Thus, the dependence of the mixing and the demixing transition on processing parameters and cycle number including the undercooling behavior of the demixing transition can be investigated. This allows a new access to the nature of nucleation of the bimodal phase separation process.

MM 21.2 Tue 12:00 H38

Time-resolved investigation of the liquid-solid phase transitions in supercooled liquid Argon and Krypton — ●ALEXANDER SCHOTTELIUS¹, BJÖRN BEYERSDORFF², TIBERIO EZQUERRA³, STEPHAN ROTH², and ROBERT GRISENTI¹ — ¹Universität Frankfurt, Frankfurt am Main, Germany — ²Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany — ³Instituto de Estructura de la Materia CSIC, Madrid, Spain

We will present new experimental results imaging the crystallization process in the two Lennard-Jones liquids, Argon and Krypton, using Small Angle and Wide Angle X-Ray Scattering (SAXS and WAXS). The sample was provided by a strongly supercooled micro-liquid jet inside a low pressure environment at cooling rates of up to 10^8 K/s. Due to the fact that the axial distance of the jet to its source can be translated into time scale, we were able to obtain a full movie of the phase transition by X-Ray scattering. In particular, while most of the final solid samples displayed the expected fcc- crystal structure,

Complex magnetic intermetallics and magnetocaloric effect — ●PETER ENTEL¹ — Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

We have performed ab initio electronic structure calculations and Monte Carlo simulations of magnetic intermetallics such as Fe-Al, Fe-Rh, Ni-Mn-Ga and Ni-Mn-(In, Sn) alloys. While Fe-Al shows mictomagnetic and metamagnetic features due to disorder and defects, near-stoichiometric Ni-Mn-Ga alloys show magnetic-field induced strain (MFIS), as the external magnetic field can drive the variant boundaries to move so that the magnetic easy axis is aligned parallel to the magnetic field direction. The other unusual type of ferroic shape-memory alloys like Ni-Mn-(In, Sn) (showing large magnetocaloric effects) leads to strongly frustrated magnetic behavior because of competing ferro- and antiferromagnetic interactions, where the parent phase shows considerably larger magnetization than the martensitic phase leading (in difference to Ni-Mn-Ga) to magnetic field-induced transformation (MFIT), namely a metamagnetic phase transition from martensite to austenite with increasing magnetic field. The related magnetostructural transition leads to the kinetic arrest phenomenon at a critical temperature where the entropy difference between austenitic and martensitic phases and the driving force for further transformation vanish (which, alternatively has been assigned to a Kauzmann point). In addition, we find transitions to supercooled austenite and unfrozen strain glass and to a cluster-spin glass. We argue that this complexity originates from the ferroic frustration and noncollinear magnetism.

15 min. coffee break

the WAXS diffraction patterns provide evidence of a hcp- structured crystal fraction for both Systems, Argon and Krypton.

MM 21.3 Tue 12:15 H38

Microstructure development of aluminum based alloys in additive manufacturing revealed from differential fast scanning calorimetry and metallographic studies — ●BIN YANG¹, OLAF KESSLER², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Rostock, Germany — ²Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Rostock, Germany

To obtain the desired additive manufacturing (AM) fabricated aluminum-based alloy parts, the rapid solidification processes need to be investigated in-situ. Based on the calorimetric method (differential fast scanning calorimetry) developed for the study of metal particles, the solidification process of aluminum-based alloy powder-particles, i.e. AlSi10Mg, was studied, for the very first time, under AM relevant heating and cooling rate conditions. A preliminary series of DFSC heating and cooling experiments was conducted, applying cooling rates as high as 80,000 K/s. The differential fast scanning calorimeter traces revealed that the material undergoes a two-stage melting and solidification processes depending on heating and cooling rates. In particular, the solidification structure of the real time quenched single droplet was observed and analyzed with focused ion beam (FIB), scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). This research proposed a new approach to research the solidification structure of single aluminum-based alloys particles used in AM technologies with precisely controlled size and extreme cooling rate.

MM 21.4 Tue 12:30 H38

Pressure-induced spin transition of Fe²⁺ in magnesio-siderite solid solution and siderite studied by x-ray Raman scattering — ●CHRISTOPHER WEIS¹, CHRISTIAN STERNEMANN¹, MAX WILKE^{2,3}, VALERIO CERANTOLA⁴, CHRISTOPH J. SAHLE⁵, GEORG SPIEKERMANN^{2,6}, YURY FOROV¹, HENDRIK RAHMANN¹, and METIN TOLAN¹ — ¹Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, GER — ²GeoForschungsZentrum(GFZ), 14473 Potsdam, GER — ³Universität Potsdam, 14469 Potsdam, GER — ⁴Bayerisches Geoinstitut, 95440 Bayreuth, GER — ⁵ESRF, 38043

Grenoble Cedex 9, FRA — ⁶DESY, 22607 Hamburg, GER

Owing to the low solubility of carbon in Earth mantle silicate phases, carbonate minerals may form as evidenced by inclusions found in diamonds formed in the Earth's mantle. Here, Siderite (FeCO₃) forms a complete solid solution with magnesite (MgCO₃). Pressure-induced high-spin (HS) to low-spin (LS) transitions of such carbonates at conditions of the inner Earth and the associated change of its magnetic properties largely influences the materials characteristics such as sound velocity and density. In contrast to diffraction experiments, high-pressure optical Raman studies found indication for the coexistence of HS and LS state in a transition range in siderite as well as in the solid solutions. We investigated the spin transition of a siderite and magnesio-siderite single crystal for pressures up to 50 GPa using diamond anvil cell by x-ray Raman scattering at the iron M_{2,3}-edge and L_{2,3}-edge. The course of the spin transition will be discussed and confronted with optical Raman, x-ray emission and Mössbauer studies.

MM 21.5 Tue 12:45 H38

Confocal Raman microscopy for noncontact and nondestructive characterization of carbon fibers — ●SERGEJ SHASHKOV, VALERY KOPACHEVSKY, ALEXANDER GVOZDEV, and ALEXANDER GRIGORENKO — SOL instruments LTD., Minsk, Belarus

Confocal Raman microscopy is a nondestructive technique in materials characterization that provides valuable structural information, and allows monitoring changes in molecular bond structure. In this paper, confocal Raman microscopy with high spatial resolution and high

sensitivity has been used for carbon fiber research. We present Raman measurement results of several types of carbon fibers. The graphitization level of fibers has been estimated.

MM 21.6 Tue 13:00 H38

Anharmonic quantum nuclear vibrations and the stability of hexagonal ice — EDGAR ENGEL, ●BARTOMEU MONSERRAT, and RICHARD NEEDS — TCM Group, Cavendish Laboratory, 19 JJ Thomson Avenue, Cambridge, CB3 0HE, UK

We use a recently developed vibrational self-consistent field approach in conjunction with first-principles density functional theory (DFT) calculations to calculate anharmonic quantum nuclear vibrations in the hexagonal and cubic forms of water ice. The very similar free energies of hexagonal and cubic have so far prevented even state-of-the-art first-principles quantum mechanical calculations using non-local DFT and quantum Monte Carlo methods from reproducing, let alone explaining, the stability of hexagonal ice. We show that, although the static lattice and harmonic vibrational energies are almost identical, anharmonic vibrations crucially stabilise hexagonal ice compared with cubic ice by at least 1.4 meV/H₂O, in agreement with experimental estimates. The difference in anharmonicity arises predominantly from the difference in vibrational frequencies of the O-H bond stretching modes, which is in agreement with recent IR absorption measurements for stacking disordered ice. We account for proton-disorder and relate our results to recent IR absorption measurements for partially proton-ordered cubic ice. Moreover, we trace the difference in anharmonicity back to the difference in structure.

MM 22: Topical session: Integrated computational materials engineering for design of new materials V

Time: Tuesday 11:45–13:30

Location: H39

MM 22.1 Tue 11:45 H39

Structure prediction of bulk materials via compressed sensing — ●RUNHAI OUYANG, LUCA M. GHIRINGHELLI, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

Structure prediction of materials from only their chemical compositions can greatly accelerate the novel material discovery and design. Fast structure prediction can be made by building a structure map based on available knowledge from material database. The key for accurate prediction is to identify the physical parameters (descriptor) that determine the material structures. While most of the current methods experience the problem of a biased intuitive feature selection or having difficulty in solving ill-conditioned linear systems when considering a big feature space, we employ the rather recent compressed sensing theory from signal and image processing field for the descriptor identification. Here, we focus on the prediction of crystal structure of ternary semiconductors and insulators with covalent and ionic bonding by building a map on which the structures are classified. Machine learning is performed on first-principle materials data from the NoMaD repository (<http://nomad-repository.eu>), complemented by newly performed density-functional calculations. We show how a physically interpretable descriptor can be identified unbiasedly and systematically by using the least absolute shrinkage and selection operator (LASSO) method from a big feature space (size n) but with a relatively small sample data set (size m , $m \ll n$).

MM 22.2 Tue 12:00 H39

Sampling parameter sensitivities for kinetic Monte Carlo models — MAX J. HOFMANN², FELIX ENGELMANN³, and ●SEBASTIAN MATERA¹ — ¹FU Berlin, Germany — ²U Stanford, USA — ³TU München

We present a three-step procedure for the sampling of local sensitivities (parameter gradients) from kinetic Monte Carlo models, which severely reduces the computational cost compared with standard numerical differentiation. In the first step, we utilize the Relative Entropy Method[1] for obtaining upper/lower bounds for the derivatives and discard those parameters with vanishing sensitivity. For the remaining, we sample the derivatives from a single trajectory employing an estimator based on Linear Response Theory. It turns out that some sensitivities can very well be sampled, while others show a higher variance. Only for the later, we perform a numerical differentiation using

Coupled Finite Differences (CFD)[2]. We demonstrate the approach by revisiting the sensitivity analysis of the CO oxidation on RuO₂ (110)[3]. We find that CFD is only necessary for a small fraction of the sensitivities. [1] Y. Pantazis and M. A. Katsoulakis, *J.Chem. Phys.* 138 (2013): 054115; [2] D. F. Anderson, David, *SIAM J. Num. Analysis* 50 (2012): 2237-2258; [3] H. Meskine, S. Matera, M. Scheffler, K. Reuter, K., H. Metiu, (2009). *Surf. Sci.*, 603 (2009): 1724-1730

MM 22.3 Tue 12:15 H39

An adaptive sparse grid approach for quantifying the error propagation in first principles kinetic Monte Carlo models — ●SANDRA DÖPKING¹, DANIEL STROBUSCH², CHRISTOPH SCHEURER², and SEBASTIAN MATERA¹ — ¹FU Berlin, Germany — ²TU München, Germany

First principles kinetic Monte Carlo (1p-kMC) models utilize Density Functional Theory (DFT) based rate constants (RCs) as the input for stochastic mesoscopic reactivity models. Despite the success of DFT, the employed approximations can easily lead to uncertainties in the RCs of two orders of magnitude. We quantify the error propagation to the 1p-kMC simulation results by a global sensitivity analysis (GSA), i.e. we decompose the error in the result into contributions caused by each uncertain RC. The required high dimensional integrals over the space of the RCs are numerically evaluated using locally and dimension-adaptive sparse grids. With this approach, we can exploit that, typically, strongly non-linear behavior only appears in small sub-domains (local adaptivity) and on low-dimensional subspaces (dimension-adaptivity) of the whole parameter space. As a prototypical example, we consider the 1p-kMC model for the CO oxidation on a RuO₂(110) surface. Comparing with local (linear) sensitivity analysis, we find qualitative differences between both approaches, but also in the global setting only a small portion of all RCs has an impact at all. Possible applications of the approach are the reduction of the number of expensive first principles simulations or the identification of descriptor sets in computational materials screening.

MM 22.4 Tue 12:30 H39

Machine Learning of the (Meta-)Stability of Octet Binaries — ●EMRE AHMETCIK, CHRISTIAN CARBOGNO, LUCA M. GHIRINGHELLI, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

Statistical learning is regarded as the most promising technique to ac-

celerate and systematically facilitate insights into computational material science. For instance, this has been recently successfully demonstrated by using compressed sensing techniques to predict the relative stability of zincblende versus rocksalt octet binary materials from the properties of the atomic constituents alone [1]. For an application in practical material science, it is however uncertain to which extent these approaches can be generalized, e.g., to predict metastable polymorphs or thermodynamic properties. To clarify this question, we have computed the relative stability of octet binaries for several different (meta-)stable crystal structures. We discuss the applicability of statistical learning for this question, how the approach can be generalized to predict thermodynamic properties such as transition pressures, and demonstrate its robustness with respect to numerical parameters. In particular, we critically discuss to which extent further data, e.g., dimeric and/or thermodynamic descriptors, are necessary.

[1] L. M. Ghiringhelli et. al., Phys. Rev. Lett. 114, 105503 (2015).

MM 22.5 Tue 12:45 H39

Automated calculations for charged point defects in MgO and $\alpha-Fe_2O_3$ — ●SUDARSAN SURENDRALAL, MIRA TODOROVA, and JÖRG NEUGEBAUER — Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

The power of modern supercomputers with efficient electronic structure codes allows the rapid screening of huge numbers of systems and properties. A prerequisite for such calculations are user-friendly high-level programming interfaces that provide highly flexible automated computational tools which assist the user, for example, in setting-up or post-processing calculations, facilitate archiving a targeted accuracy or high-throughput screening of materials. Using concepts of modern object oriented programming and database management we have developed *PyIron*, a robust computational materials python library. The capabilities of *PyIron* will be demonstrated and discussed using the automation of charged point defects calculations for MgO and $\alpha-Fe_2O_3$. Our density functional theory calculations are performed using the semi-local GGA functional for MgO and the GGA+U approach for $\alpha-Fe_2O_3$. The FNV finite supercell charge correction [1] is applied to correct for spurious interactions resulting from the use of periodic boundary conditions. Subtleties of its automated application, the effect of the Coulombic interaction parameter U has on the band gap of $\alpha-Fe_2O_3$ and on the defects' thermodynamics, will be discussed.

[1] C. Freysoldt, J. Neugebauer, and C. G. Van De Walle, Phys. Rev. Lett. 102, 016402 (2009).

MM 22.6 Tue 13:00 H39
Ab initio materials design — SILVANA BOTTI¹ and ●MIGUEL MARQUES² — ¹Friedrich-Schiller University of Jena, Germany — ²Martin-Luther University of Halle-Wittenberg, Germany

One of the most exciting developments in condensed matter over the past years is, without doubt, materials design. This new discipline aims at solving the called inverse problem: given a certain desired property (or properties), discover (design) the material that possesses this property under a given set of constraints. These constraints can be related to the mechanical or chemical stability of the compounds, their price, their availability, etc. The target properties can be related to applications, e.g., in photovoltaics, batteries, etc.

Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, which make them suitable tools for predicting electronic properties of “real” materials. Thanks to the availability of supercomputers, the powerful combination of theoretical spectroscopy with high-throughput calculations and structural prediction allows to explore the periodic table in search of new materials, providing a precious starting point for further experimental studies.

MM 22.7 Tue 13:15 H39

Bonding and electron-phonon interaction in high- T_c hydrides — ●CHRISTOPH HEIL and LILIA BOERI — University of Technology Graz

High-temperature superconductivity in hydrogen-rich compounds has been predicted by Ashcroft almost 50 years ago [1], yet was only recently observed in experiments by Drozdov et al. [2], who measured a critical temperature above 190 K in hydrogen-sulfide at 200 GPa pressure. In a similar experiment, the same group reported a T_c of 100 K in pressurised phosphine [3].

In this talk, I will show that the record-breaking T_c in H_3S does not originate from the heavier atoms exerting pressure on the hydrogen lattice, but that it is due to the formation of unusually strong polar covalent bonds, stabilised under extreme pressures. I will discuss the bonding, electron-phonon coupling and the superconducting properties of sulfur-hydrides and highlight possible routes to realise similar bonding conditions in other hydrogen-rich compounds [4].

[1] N.W. Ashcroft, Phys. Rev. Lett. 21, 1748 (1968)

[2] A.P. Drozdov, M.I. Eremets and I.A. Troyan, Nature 525, 73 (2015)

[3] A.P. Drozdov, M.I. Eremets and I.A. Troyan, arXiv:1508.06224

[4] C. Heil and L. Boeri, Phys. Rev. B 92, 060508(R) (2015)

MM 23: Mechanical Properties II

Time: Tuesday 11:45–13:15

Location: H52

MM 23.1 Tue 11:45 H52

Dislocation structure and ordering effects in high entropy alloys — ●LEONIE KOCH, ALEXANDER STUKOWSKI, and KARSTEN ALBE — FG Materialmodellierung, FB Materialwissenschaft, Technische Universität Darmstadt, Germany

High entropy alloys, mixtures of least five elements, have recently attracted considerable attention in the field of high-performance materials. It is assumed that a high configurational entropy stabilizes solid solution states at low temperatures and simultaneously avoids the formation of brittle intermetallic phases. These structural simple solid solutions exhibit a considerable strength, while preserving sufficient ductility. Nevertheless, there has been some disagreement about the high entropy effect on phase formation and stability and chemical ordering instabilities in N -component alloys have not yet been clarified for a variety of alloy systems. Therefore, we investigate the competing effects of entropy and enthalpy with decreasing temperatures by using variance-constraint semi-grand canonical Monte Carlo simulations and subsequently quantify short-range order. We further show how inherent lattice strains in atomic-scale composites affect dislocation motion under external stress at different temperatures.

MM 23.2 Tue 12:00 H52

Embryonic cracks at grain boundaries in bcc W and Fe: an atomistic study — ●JOHANNES J. MÖLLER and ERIK BITZEK — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute I, Erlangen, Germany

Advancing our understanding of grain boundary (GB) fracture is key for a variety of engineering problems spanning from brittle intergranular fracture of polycrystalline components to the failure of micro-electromechanical devices at single GBs. GB cracks are often assumed to be infinitely long and straight. At the very beginning of their existence, however, embryonic cracks are of nano-scale dimensions and have strongly curved crack fronts. Until now, the effect of crack-front curvature on the elementary crack-tip processes has not been studied in detail.

Here, we report on our recent large-scale molecular dynamics simulations of penny-shaped cracks at five GBs in the bcc metals W and Fe. The observed crack-tip processes ranged from purely brittle bond breaking to purely ductile emission of deformation twins. The evolution of crack-tip plasticity is characterized by dislocation emission from growing twins and transmission of the nucleated dislocations through GBs. Our simulations indicate that the initial fracture event at penny-shaped crack fronts can be predicted by analyzing the results for straight cracks. The characteristic crack-tip processes, on the other hand, were not observed in such quasi-2D simulations. This highlights the importance of 3D modeling of cracks to obtain a deeper mechanistic understanding of the ongoing crack-tip processes.

MM 23.3 Tue 12:15 H52

Push-Out Verhalten von Wolfram-Faserverstärktem Wolfram — ●BRUNO JASPER¹, STEPHAN SCHÖNEN², JAN W. COENEN¹, TILL HÖSCHEN³, JOHANN RIESCH³, RUDOLF NEU^{3,4} und CHRISTIAN

LINSMEIER¹ — ¹FZ Jülich GmbH, IEK4 - Plasmaphysik, Jülich, GER — ²FZ Jülich GmbH, ZEA1 - Engineering und Technologie, Jülich, GER — ³IPP, Garching, GER — ⁴TU München, Garching, GER

Mit seinen vorteilhaften Eigenschaften im Bezug auf z.B. Wasserstoffrückhaltung oder Erosion durch Plasma ist Wolfram (W) ein Kandidat für Komponenten für die erste Wand zukünftiger Fusionskraftwerke. Der große Nachteil bei der Verwendung von W besteht jedoch in seiner hohen Spröd-Duktil Übergangstemperatur. Um diesen Nachteil zu umgehen wird ein Wolfram-Faserverstärkter Wolfram (W_f/W) Kompositwerkstoff entwickelt. Dieser besteht aus einem, mit einer Zwischenschicht (Interface) versehenen, W-Draht und einer W-Matrix. Wird ein Riss im Material initiiert, ist es auf Grund des Interfaces möglich, dass extrinsisch-zähigkeitssteigernde Mechanismen wirken können. Somit wird die Risspitzenenergie reduziert und ein pseudo-duktilen Verhalten erreicht.

Um ein besseres Verständnis dieser Mechanismen auf mikroskopischer Ebene aufzubauen wurden umfangreiche Push-Out Tests an dünnen Einzelfaser W_f/W Proben durchgeführt. Die experimentellen Ergebnisse, welche den Einfluss von Probengeometrie, Probenherstellung und Versuchsaufbau beleuchten, werden mit entsprechenden Simulationsarbeiten verglichen und vorgestellt.

MM 23.4 Tue 12:30 H52

Sequence of microstructure evolution processes in steel under tribological loading — ●CHRISTIAN GREINER, KARSTEN WOLFF, DANIEL BRAUN, ZHILONG LIU, and JOHANNES SCHNEIDER — KIT, Kaiserstrasse 12, 76131 Karlsruhe

The exact evolution of a material's microstructure under tribological loading is of great importance for both materials physics and tribology. There is however a significant lack of knowledge about the elementary mechanisms of microstructure evolution under tribological load as well as their kinetics. Therefore, the microstructure evolution of steel C85 pellets sliding against steel 100Cr6 disks is characterized after different numbers of acceleration-deceleration cycles. Focused ion beam cross-sections are prepared along the sliding direction. Two tribologically modified surface layers are found: One with bent grain boundaries and one of nanocrystalline nature. We hypothesize that the second layer is formed by breaking down the most bent regions of the first one when a critical grain boundary bending angle is reached and then consumes it from the top. A model originally developed for High Pressure Torsion (HPT) was successfully applied to estimate the thickness of the fine-grained layer and the applied shear strain.

MM 23.5 Tue 12:45 H52

How ligament connectivity determines stiffness of nanoporous gold? — ●BAO-NAM NGÔ^{1,2}, BENEDIKT ROSCHNING³, ALEXANDER STUKOWSKI², JÜRGEN MARKMANN^{1,3}, KARSTEN ALBE², and JÖRG WEISSMÜLLER^{1,3} — ¹Institut für Werkstofforschung, Werk-

stoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Darmstadt, Germany — ³Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

We present a study of the deformation-induced changes of ligament connectivity and its influence on the elasticity of nanoporous gold - a promising material for applications in actuation, catalysis and sensing, as well as a model candidate for study of mechanics at the nanoscale. Using molecular dynamics, a computer sample created by spinodal decomposition was uni-axially deformed in a load/unload sequence. A surface reconstruction algorithm was employed to provide necessary information for calculating genus density and its changes during the plastic deformation. The results were then cast against corresponding changes of the elastic modulus. We also performed Finite Element Analysis on some deformed structures, using the reconstructed surfaces as initial structures in order to get a reference which is not influenced by size and interface effects. While our study reveals a strong influence of the ligament connectivity on the elastic behavior of nanoporous gold, other factors must be taken into account to explain its exceedingly compliant behavior.

MM 23.6 Tue 13:00 H52

Correlation between elasticity and stability in refractory alloys — ●SANDRA HOPPE¹, SASCHA B. MAISEL², and STEFAN MÜLLER¹ — ¹Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ²Max-Planck Institut für Eisenforschung, Düsseldorf, Germany

Varying an alloy's concentration or alloying constituents strongly influences its structural and mechanical properties. Modern simulation methods like density functional theory (DFT) in combination with the cluster expansion (CE) make the whole configuration space accessible. Recent results for several face-centered cubic (fcc) binary metal alloys [1] suggest a linear correlation between thermodynamic stability and elastic properties at a fixed stoichiometry. This study aims to investigate the generality of these findings by considering a similar correlation for the binary body-centered cubic (bcc) refractory alloy systems Ta-W and Mo-Nb. For this purpose, formation enthalpies as well as the symmetrically averaged elastic constants c_{11} and c_{44} are expanded via a CE fit with DFT input. Interestingly, the shear constant c_{44} shows an opposing trend to that observed for fcc alloys in certain concentration regimes. This phenomenon is discussed with regard to an anomalous behavior of c_{44} with varying alloy concentration, temperature or pressure [2,3].

[1] S. B. Maisel, M. Höfler, and S. Müller. *Nature* **491** (2012) 740.

[2] K. W. Katahara *et al.* *J. Phys. F: Met. Phys.* **9** (1979) 773.

[3] C. E. Anderson and F. R. Brotzen. *J. Appl. Phys.* **53** (1982) 292.

MM 24: Topical session: Caloric Effects in ferroic materials II - Methods and Applications

Time: Tuesday 11:45–13:15

Location: H53

15 min. coffee break

MM 24.1 Tue 12:00 H53

Detailed loss analysis of a magnetocaloric demonstrator using FEM-simulations — ●DIMITRI BENKE, TINO GOTTSCHALL, FABIAN JÄGER, MARC PABST, KONSTANTIN SKOKOV, ILIYA RADULOV, and OLIVER GUTFLEISCH — TU Darmstadt, Institute of Material Science, Alarich-Weiss-Str. 16, 64287 Darmstadt, Germany

The performance of many magnetocaloric materials has been reported and compared many times in the literature [1-3]. However, this comparison is mostly not done in conditions mirroring the real device. In order to assess materials in an environment being comparable to application, a magnetocaloric test bench was built. This demonstrator can be used to compare the performance of a material under cyclic conditions being in contact with an oscillating heat exchange fluid.

In order to assess the suitability of a material, the different loss mechanisms during operation of the demonstrator have to be evaluated. By this it is possible to make full use of the potential of the materials. This has been done by combining measurements of the temperature span and FEM simulations of the magnetocaloric test bench when varying the system parameters.

This work was supported by the Darmstadt Graduate School of Ex-

cellence Energy Science and Engineering.

[1] M.E. Wood, W.H. Potter, *Cryogenics* Vol. 25, Issue 12, (1985) 665.

[2] K.G. Sandeman, *Scripta Mater.* **67** (2012) 566.

[3] D.D. Belyea *et al.*, *Sci. Rep.* **5** (2015) 15755.

MM 24.2 Tue 12:15 H53

In-situ XRD and 3D imaging techniques for the study of magnetocaloric materials — ●ANJA WASKE^{1,2}, ALEXANDER FUNK^{1,2}, KAI SELLSCHOPP^{1,2}, ALEXANDER RACK³, and SEBASTIAN FÄHLER^{1,2} — ¹IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — ²Institute for Materials Science, TU Dresden, Helmholtzstraße 7, 01069 Dresden, Germany — ³ID 19, ESRF, 6 rue Jules Horowitz, 38043 Grenoble Cedex, France

In magnetocaloric La(Fe,Si)13, an isostructural first-order transition connected with a volume change of around 1.5 vol.% occurs at the critical temperature T_t . We use in-situ computed tomography and situ X-ray diffraction to study this magnetovolume transition as a function of temperature. The experiments have been carried out at the beamline ID 19 at the ESRF in Grenoble (tomography) and the Petra III /2.1 beamline at DESY in Hamburg, respectively. We show that i) by 3D imaging it is possible to track the magnetovolume transition, ii) nucleation and growth of the ferromagnetic phase depends

strongly on surface morphology and iii) the virgin effect in magnetocaloric La(Fe,Si)₁₃ is connected to the formation of cracks [1]. These findings connect microstructural aspects of the first-order transition to important properties like hysteresis and kinetics of the phase transition and can therefore help to tailor magnetocaloric materials towards application. Funded by DFG through SPP 1599 www.FerroicCooling.de. [1] A. Waske et al., PSS-RRL 9 (2) 136-140 (2015)

MM 24.3 Tue 12:30 H53

Direct vs indirect Monte-Carlo methods for calculating the electrocaloric effect — ●CONSTANZE KALCHER, ALEXANDER STUKOWSKI, and KARSTEN ALBE — FG Materialmodellierung, FB Materialwissenschaft, Technische Universität Darmstadt, Germany

Conventionally, the electrocaloric effect is determined indirectly by integrating Maxwell's relation. However, a number of approximations are usually made during the process, such as assuming a constant heat capacity. In this contribution we want use a computer model to show to what extent these approximations affect the resulting adiabatic temperature change and how to eliminate possible error sources. Therefore we present three Monte-Carlo methods: (a) Metropolis, (b) Wang-Landau and (c) Creutz, that allow to calculate the adiabatic temperature change of the electrocaloric effect on a 2 dimensional 4-state Ising model. We show that both the direct and indirect approach lead to the same result, but for the indirect route great care has to be taken when performing the numerical integration over the pyroelectric coefficients and the entropy.

MM 24.4 Tue 12:45 H53

In-situ synchrotron XRD investigation of the structural phase transition in epitaxial Ni-Mn-Ga-Co thin films on ferroelectric substrates — ●BENJAMIN SCHLEICHER^{1,2}, STEFAN SCHWABE¹, ROBERT NIEMANN^{1,2}, ANETT DIESTEL¹, ANJA WASKE¹, RUBEN HÜHNE¹, PETER WALTER^{3,4}, LUDWIG SCHULTZ^{1,2}, KORNELIUS NIELSCH¹, and SEBASTIAN FÄHLER^{1,2} — ¹IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — ²TU Dresden, Institute for Solid State Physics, D-01062 Dresden, Germany — ³Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg, Germany — ⁴2nd Institute of Physics B and JARA-FIT, RWTH Aachen University, D-52047 Aachen, Germany

For solid-state refrigeration, the phase transition in Ni-Mn-Ga-Co

can not only be influenced by magnetic fields, but also by mechanical stress. This can be achieved by straining an epitaxial magnetocaloric thin film via a ferroelectric substrate. We investigated sputter deposited epitaxial Ni-Mn-Ga-Co thin films on ferroelectric Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O₃ (PMN-PT) substrates. Temperature dependent texture and magnetic measurements show the structural and magnetic phase transition in the material. In-situ synchrotron XRD measurements on the P02.1 beamline at PETRA III (DESY, Hamburg) have been used to demonstrate the influence of mechanical stress on the phase transition by in-situ application of an electric voltage to the multiferroic stack and a temperature-strain phase diagram was obtained. Funded by DFG through SPP 1599 www.FerroicCooling.de.

MM 24.5 Tue 13:00 H53

Magnetocaloric properties of freestanding and substrate-constrained Ni-Mn-Ga-Co films — ●ANETT DIESTEL^{1,2}, ROBERT NIEMANN¹, BENJAMIN SCHLEICHER¹, STEFAN SCHWABE^{1,2}, LUDWIG SCHULTZ^{1,2}, and SEBASTIAN FÄHLER¹ — ¹IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — ²TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

Ferroic cooling processes that rely on field-induced first-order transformations of solid materials are a promising step towards a more energy-efficient refrigeration technology. In particular thin films are discussed for their fast heat transfer and possible applications in microsystems. They can be used as model systems to understand the transformation mechanism. We analyze the martensitic transformation in substrate-constrained and freestanding epitaxial Ni-Mn-Ga-Co films. By means of M(T) and M(H) measurements in vicinity of the phase transformation, we compare entropy changes and field-temperature phase diagrams, which differ only slightly depending on the scanning parameter. These effects are related to the vector character of a magnetic field, which acts differently on the nucleation and growth processes compared to the scalar character of temperature. We observed an asymmetric thermal hysteresis between the ferromagnetic austenite and the ferromagnetic martensite. The sharp cooling but gradual heating branch at low magnetic fields is explained by using a microstructural model of martensitic transformation describing energy barriers of nucleation and growth processes. This work was funded by the DFG SPP1599.

MM 25: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I

Time: Tuesday 14:00–16:00

Location: H24

Topical Talk

MM 25.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — ●SHUICHI MURAKAMI — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z₂ topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

MM 25.2 Tue 14:30 H24

Topological orbital magnetic moments — ●MANUEL DOS SANTOS DIAS, JUBA BOUAZIZ, MOHAMMED BOUHASSOUNE, STEFAN BLÜGEL, and SAMIR LOUNIS — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic

spin textures, even without SOI, justifying the 'topological' label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

MM 25.3 Tue 14:45 H24

The orbital Rashba effect — ●DONGWOOK GO^{1,2}, PATRICK BUHL¹, GUSTAV BIHLMAYER¹, YURIY MOKROUSOV¹, HYUN-WOO LEE², and STEFAN BLÜGEL¹ — ¹Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — ²Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\text{orb-R}}(\mathbf{k}) = \alpha_{\text{orb-R}} \mathbf{L} \cdot (\hat{\mathbf{z}} \times \mathbf{k})$, where \mathbf{L} is the orbital moment derived from atomic orbitals and $\alpha_{\text{orb-R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the \mathbf{k} -space. The mechanism behind the emergence of the $H_{\text{orb-R}}(\mathbf{k})$ can be understood as the \mathbf{k} -dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect

is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag *s*-orbital and a Bi *p*-orbital leads to the orbital Rashba effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

MM 25.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — ●JUBA BOUAZIZ, MANUEL DOS SANTOS DIAS, PHIVOS MAVROPOULOS, STEFAN BLÜGEL, and SAMIR LOUNIS — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinskii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].

[1] J. Bouaziz *et al.* in preparation.

[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

MM 25.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — ●IMARA L. FERNANDES, BENEDIKT SCHWEFLINGHAUS, JUBA BOUAZIZ, STEFAN BLÜGEL, and SAMIR LOUNIS — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).

[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79**

(2014).

[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).

[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

MM 25.6 Tue 15:30 H24

Topological magnons: Any chance to find them? —

●ALEXANDER MOOK¹, JÜRGEN HENK², and INGRID MERTIG^{1,2} —

¹Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle —

²Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., Lu₂V₂O₇, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe₃Sn₂ as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang *et al.*, PRB **87**, 144101 (2013); [2] A. Mook *et al.*, Phys. Rev. B **89**, 134409 (2014); *idem*, Phys. Rev. B **90**, 024412 (2014); *idem*, Phys. Rev. B **91**, 224411 (2015); *idem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell *et al.*, Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose *et al.*, Science **329**, 297 (2010).

MM 25.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory —

●MATHIAS C.T.D. MÜLLER, CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the *T*-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ . We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

MM 26: Poster session II

Posters should be displayed by 4 pm. The MM poster price will be awarded during the annual general assembly on Wednesday evening.

Posters submitted to: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science, Electron Microscopy of Materials, Interfaces, Functional Materials, Nanomaterials, Caloric Effects in ferroic materials

Time: Tuesday 18:30–20:30

Location: Poster B3

MM 26.1 Tue 18:30 Poster B3

Mechanical behavior of fivefold twinned silver nanowires by means of *in situ* tensile tests in the TEM — ●NADINE SCHRENKER¹, MIRZA MACKOVIC¹, MANUELA GÖBELT², SILKE CHRISTIANSEN^{2,3}, and ERDMANN SPIECKER¹ — ¹Center for

Nanoanalysis and Electron Microscopy, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — ²Max Planck Institute for the Science of Light, Erlangen, Germany — ³Helmholtz Centre Berlin for Materials and Energy, Germany

Organic (opto)electronics have recently undergone a rapid development. Major advantages compared to their inorganic counterparts are that they can be manufactured on flexible substrates. Silver nanowire (Ag NW) films are highly promising as flexible transparent electrodes, e.g., for organic solar cells, as they fulfill the requirement of a low sheet resistance combined with a high transparency. Indium tin oxide (ITO), which is still the most common used material, behaves brittle under deformation and is relatively expensive. On a macroscopic scale bending tests revealed the excellent performance of Ag NW films, since the increase of resistance is small compared to ITO films. To complement the macroscopic bending tests, understand failure mechanisms and prospectively optimize the deformation behavior of AgNW electrodes *in situ* mechanical testing in the TEM are conducted. On a nm scale tensile tests of single 5-fold twinned Ag NWs show a ductile behavior and a size effect of the strength. Moreover, microscopic *in situ* tensile tests of individual junctions and areas on the μm scale of AgNW films in the TEM are in focus of our current research.

MM 26.2 Tue 18:30 Poster B3

Surface Nucleation Controlled Plasticity in Twinned Gold Nanowires — ●ZHUOCHENG XIE, JAKOB RENNER, ARUNA PRAKASH, and ERIK BITZEK — Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials Science & Engineering, Institute I, Erlangen, Germany

Metallic nanowires (NWs) receive currently much attention due to their often superior mechanical properties compared to bulk materials. Similarly, nanotwinned metals have lately attracted a lot of interest because they combine high strength with high ductility, two properties which have been thought to be mutually exclusive. Recently, nanotwinned nanowires were reported, which could combine both strengthening mechanisms, namely surface dislocation nucleation controlled plasticity and hardening due to dislocation - twin interactions.

Here, we report on molecular dynamics simulations of tensile tests on single and multi-twinned Au nanowires with $\langle 110 \rangle$ and $\langle 112 \rangle$ orientations. The interactions of partial dislocations nucleated at the surfaces with the twin boundaries parallel to the wire axis are analyzed in detail and the resulting deformation behavior is compared to recent experiments.

MM 26.3 Tue 18:30 Poster B3

Investigation of perovskite interfaces with negative spherical aberration in HRTEM — ●TOBIAS MEYER¹, PATRICK PERETZKI¹, BENEDIKT IFLAND², CHRISTIAN JOOSS², and MICHAEL SEIBT¹ —

¹IV. Physical Institute, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²Institute for Materials Science, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The well-known Shockley-Queisser limit for the efficiency of single junction solar cells is based on energy losses due to transmission of low energy photons and thermalization of highly excited charge carriers. To overcome these limitations semi-conductors with small band gaps and long relaxation times are desirable. Long living states of small polarons have been observed in strongly correlated perovskite materials of the general form $A_{1-x}A'_xB\text{O}_3$. The properties of these systems are related to orbital, charge and magnetic ordering phenomena which are highly dependent on the doping level and the particular choice of A , A' , and B . In the perfect perovskite lattice the B -site ion is centered in an octahedral spanned by the surrounding oxygen anions. Cooperative distortions and tilts of the octahedral affect the ordering phenomena and can also lead to relaxations of e.g. epitaxial strain. Junctions between $\text{Pr}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ (PCMO) and SrTiO_3 (STO) have been investigated in an image corrected TEM using negative spherical aberration imaging (NCISI) combined with focal series recording. Object waves reconstructed from such focal series were processed to study oxygen vacancies as well as octahedral tilts and distortions induced by the slightly different lattice parameters of PCMO and STO.

MM 26.4 Tue 18:30 Poster B3

Exploring the friction between atomic layers with *in situ* SEM mechanical testing — ●PETER SCHWEIZER, FLORIAN NIEKIEL, and ERDMANN SPIECKER — Center for Nanoanalysis and Electron Microscopy (CENEM), University of Erlangen-Nuremberg, Cauerstr. 6, 91058, Erlangen, Germany

With the advent of nano-electromechanical systems, the understanding of atomic-scale friction becomes very important, since the life-time and functionality of such systems is often limited by the effects of friction and wear. Interfaces made of flat atomic layers can in certain conditions show the effect of ultra-low friction, also referred to by the term of

“superlubricity”, which might alleviate the tribological problems that NEMS face today. However there are still a lot of open questions regarding friction on the atomic scale, especially the evolution of the microstructure in an interface during sliding.

In this work we present an approach to quantitatively measure the friction forces between atomic layers, using vanadium diselenide (VSe_2) as a model system. Following a preparation routine with the focused ion beam area dependent friction forces are measured *in situ* in the scanning electron microscope with the help of a micro-manipulator and a spring table. The microstructure of the interface is analyzed after sliding using transmission electron microscopy. Different crystallographic orientations of the tribological interface are compared and links to the microstructure are drawn.

MM 26.5 Tue 18:30 Poster B3

Self-assembly of an imidazole-based ligand on Au(111) and on Cu(111) — ●PATRICK SEITZ¹, NICO FRITSCH², THOMAS

WAIDMANN², NICOLAI BURZLAFF², and SABINE MAIER¹ —

¹Department of Physics, FAU Erlangen-Nürnberg, Germany —

²Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany

Imidazole-based ligands are versatile building blocks to form one-dimensional coordination polymers on surfaces [1,2]. In this work, the self-assembly and conformation of 1,2-bis(*N*-methylimidazol-2-yl)ethylene ligands on Au(111) and Cu(111) was studied using low temperature scanning probe microscopy (STM) in ultra-high vacuum. The subtle balance between intermolecular and molecule-surface interactions determines, whether the molecules adsorb as *cis*- or *trans*-isomers. On Au(111), the molecules interact with one another through hydrogen bonds. We observe dimers and trimers formed from *cis*-isomers while *trans*-isomers self-assemble in one-dimensional chains at submonolayer and two-dimensional islands at monolayer coverage. In contrast, the molecules preferably adsorb as monomers on Cu(111) owing to a strong molecule-surface interaction. [1] Fischer et al., Chemistry - A European Journal, 2011, 17 (34), 9293-9297 [2] Fritsch et al., Inorganic Chemistry, 2014, 53 (23), 12305.

MM 26.6 Tue 18:30 Poster B3

Deformation behavior and solid solution strengthening of

metallic micro- and nanoparticles studied by *in situ* electron

microscopy — ●PATRICK HERRE¹, STEFAN ROMEIS¹, JONAS PAUL¹,

MIRZA MAČKOVIĆ², FLORIAN NIEKIEL², SIMON M. KRASCHEWSKI²,

ERDMANN SPIECKER², and WOLFGANG PEUKERT¹ — ¹Institute of

Particle Technology (LFG), Friedrich-Alexander-Universität Erlangen-

Nürnberg, 91058 Erlangen, Germany — ²Institute of Micro-

and Nanostructure Research (IMN), Friedrich-Alexander-Universität

Erlangen-Nürnberg, 91058 Erlangen, Germany

The small scale deformation behavior of (sub-) micron particles and structures is fairly distinct from the bulk due to internal and external interfaces as the size dimensions are close to the characteristic length scale (e.g. dislocation spacing) of the underlying physical (deformation) mechanism. In order to deepen the current understanding of small scale mechanics, metallic particles of defined size, morphology, structure and composition are synthesized by liquid and solid state dewetting of thin metallic films on ceramic substrates. As a model and reference system, thin Au films are dewetted on (0001) sapphire substrates. Hence, single-crystalline and defect-free Au particles of defined shape and orientation with respect to the substrate are obtained and depict an ideal specimen for decent mechanical testing. In addition, thin films composed of pure Ni as well as Ni-rich solid solutions of Ni-Ta and Ni-W are prepared via electron beam PVD on sapphire substrates. *In situ* electron microscopy is used as a powerful tool for conducting deformation experiments of adequate image and data resolution.

MM 26.7 Tue 18:30 Poster B3

Fracture toughness of freestanding gold thin films studied

by bulge testing — ●EVA PREISS, BENOIT MERLE, and MATHIAS

GÖKEN — Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU),

Materials Science & Engineering, Institute I, Germany

A versatile bulge test setup was used to perform mechanical tests on rectangular gold membranes with columnar microstructure and thicknesses ranging from 100 nm to 350 nm. It can be used in a conventional way to calculate stress-strain curves and determine parameters such as residual stress and plane-strain modulus. Alternatively, the setup can be inserted into an atomic force microscope (AFM) which allows *in-situ* imaging of the topography of the deforming membrane.

In order to determine the fracture toughness of thin films, narrow crack-like slits of 10 μm length were milled into the center of the membranes by focused ion beam (FIB). Subsequently, the membranes were loaded until rupture.

The fracture toughness of all tested gold films is much lower than the literature value for bulk gold. However, the fracture toughness remains constant within the investigated thickness regime. In-situ AFM scans of the crack tip region show stable crack growth before failure. Plastic deformation is localized to a narrow corridor in front of the crack tip and mainly takes place along grain boundaries.

The obtained fracture toughness values agree well with literature values for other metallic thin films. New insights from the in-situ AFM scans are discussed with regard to possible deformation mechanisms.

MM 26.8 Tue 18:30 Poster B3

In situ micromechanical testing and local strain analysis of nanoporous gold — •THOMAS PRZYBILLA, ERICH THIESS, FLORIAN NIEKIEL, BENJAMIN WINTER, MIRZA MAČKOVIĆ, and ERDMANN SPIECKER — Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy (CENEM), Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Cauerstrasse 6, 91058 Erlangen, Germany

Nanoporous gold (npg) acts as a model material to study mechanical size effects in nanostructured metals as the ligament size can be tailored within the nanometer to micrometer range. Au ligaments act together as a 3D open-porous network of interconnected nanostruts resulting in high mechanical strength under compression and nanoindentation. With decreasing ligament size stresses close to the theoretical shear strength were reported. In this work we study the mechanical behavior of npg foams with varying ligament diameter in the range of 10 to 100 nm by pillar compression experiments performed in situ via scanning electron microscopy (SEM) and transmission electron microscopy (TEM). npg pillars are prepared by focused ion beam (FIB) milling and characterized by scanning transmission electron microscopy (STEM) tomography. Taking the porosity into account the yield stress is evaluated with respect to the ligament diameter. The local strain is mapped from in situ experiments by image correlation techniques revealing local strain gradients and showing a distinct difference between local and macroscopic yield strain values.

MM 26.9 Tue 18:30 Poster B3

Plasticity of interfaces - TEM in situ indentation and atom probe microscopy on TiAl — •CAROLIN PUSCHOLT and MATHIAS GÖKEN — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Insitute I, Martensstr. 5, 91058 Erlangen, Deutschland

Interfaces in crystalline metallic materials significantly influence the material's mechanical properties. In fact, the study of the behavior of crystalline materials can often be reduced to the study of the structure and properties of their internal interfaces.

In this work Titanium Aluminides (Ti-48Al) are studied as a model system to determine the properties of interfaces since they offer a lamellar structure that represents a multilayer system made of two phases with a semi-coherent interface and a very distinct orientation relationship between the tetragonal γ -TiAl phase with its $L1_0$ structure and the hexagonal α_2 -Ti₃Al phase with an ordered $D0_{19}$ structure. This was done by in situ indentation in the transmission electron microscope where the mechanical response of the material to indentation loads can be studied in real-time which permits the direct observation of the dynamics and mechanisms of dislocation motion and dislocation-interface interactions. Further investigations to study specific interface characteristics like segregations to (misfit) dislocations or deviations from the perfect stoichiometry of intermetallic phases that also strongly influence the properties were done via atom probe microscopy as a complementary method.

MM 26.10 Tue 18:30 Poster B3

Si diffusion and precipitation in Al during the Al-induced layer exchange (AILE) process — •SIMON M. KRASCHESKI, BENJAMIN BUTZ, and ERDMANN SPIECKER — Lehrstuhl für Mikro- und Nanostrukturforschung & Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg, Erlangen, Germany

Al-induced layer exchange (AILE) is a promising route of fabrication for polycrystalline intrinsic Si seed layers from an amorphous state at low temperatures. The process makes use of the phenomenon of metal-induced crystallization and is characterized by a layer exchange in a

stack of Si/oxide/Al on glass substrate at temperatures in the range of 180-550 °C. According to the current understanding of the process, atomic Si diffuses into the Al layer where it becomes oversaturated and forms crystalline precipitates. The precipitates grow laterally (up to several 10th of μm) thus replacing the Al which is "pushed up" into the original a-Si layer. Until now no analytical SEM/TEM studies have been performed in order to verify the Si content in the Al layer during the process.

First results on *ex situ* quenched samples with Si show a vertical gradient of Si in the Al layer with a range of 2-5 at%, which is much higher than expected from the phase diagram (round about 1 at%). Additionally the Si in the Al layer distribution seems to be independent from interfaces and grain boundaries.

MM 26.11 Tue 18:30 Poster B3

Electrochemical Hydrogenography on thin Magnesium films — •NIKLAS TEICHMANN, MAGNUS HAMM, MELISSA SCHENKER, and ASTRID PUNDT — Univ. Göttingen, IMP, Friedrich- Hund-Platz 1, 37077 Göttingen, Germany

Hydrogen in metals like Magnesium changes the physical properties of the host material, such as the optical properties.[1] This is the basic idea of the Hydrogenography where the change in the transistivity and reflectivity is measured to determine locally the Hydrogen concentration.[2] At room temperature the Mg-H system has a wide miscibility gap. This leads to a strong optical contrast.

In this paper, the optical change of thin Mg-films under hydrogen uptake is investigated using an electrochemical Hydrogenography technique.[3] By this, the MgH₂ formation can be measured and the formation kinetics can be studied.

As Mg oxidizes easily, oxides can be hardly prevented. In contact with hydrogen, hydroxides appear. These oxides and hydroxides directly influence the Hydrogen uptake and therefore, their impact is planned to be minimized.

Financial support by the DFG via projects PU131/9-2 and PU131/12-1 is gratefully acknowledged.

[1] T. Richardson et al. Applied Physics Letters 78.20 (2001): 3047-3049.

[2] R. Gremaud et al. Advanced Materials 19.19 (2007): 2813-2817.

[3] J. Kürschner et al. Journal of Alloys and Compounds 593 (2014): 87-92.

MM 26.12 Tue 18:30 Poster B3

Orientation changes upon attachment of spider hairs investigated in situ using scanning X-ray nanobeam diffraction and small-angle scattering — •SILJA FLENNER¹, CLEMENS SCHABER², IGOR KRASNOV¹, STANISLAV GORB², CHRISTINA KRYWKA³, EMANUELA DI COLA⁴, MARTIN ROSENTHAL⁴, MANFRED BURGHAMMER⁴, and MARTIN MÜLLER^{1,3} — ¹Institute of Experimental and Applied Physics, Kiel University, Germany — ²Institute of Zoology, Kiel University, Germany — ³Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany — ⁴ESRF, Grenoble, France

The hairy attachment system of spiders enables these animals to walk upside-down on rough and smooth surfaces and support a multiple of the body weight without the use of glue. These outstanding biological structures comprise of pads including hundreds to thousands of specially designed hairs that are made of composite materials consisting of proteins and reinforcing chitin fibres.

The technique of high spatial resolution mapping based on scanning X-ray nanobeam diffraction and small-angle scattering was used to study the hairy attachment system of spiders. Each point of a map represents a structural parameter such as orientation or scattered intensity extracted from a diffraction pattern. This technique was combined with an in situ attachment/detachment procedure. The goal of our study is to gain an in-depth understanding of the working principle of the attachment and detachment processes of single hairs to a surface.

MM 26.13 Tue 18:30 Poster B3

X-ray Nanodiffraction for in situ Microscopy — •CHRISTINA KRYWKA^{1,2}, STEPHAN V. ROTH³, and MARTIN MÜLLER¹ — ¹Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht — ²Christian-Albrechts-Universität, Leibnizstraße 19, D-24118 Kiel — ³DESY, Notkestraße 85, D-22607 Hamburg

The origins of the macroscopic behavior of synthetic and natural high-performance materials can often be found on no less than atomic length scales. Access to these dimensions is barred for light

microscopes while electron microscopes suffer from the low penetration depth of electrons. Consequently, high resolution structural data recorded with external stimuli modified *in situ* is rare to find. X-ray nanodiffraction is able to overcome these hurdles. That's because a sub-micrometer sized hard X-ray beam can extract local structural information residing within bulk volumes and from samples inside extended sample environments - given a sufficiently long focal distance. The Nanofocus Endstation of P03 beamline (PETRA III) is a dedicated X-ray nanodiffraction setup. Tensile and indentation stresses, magnetic and electric fields, hydrostatic pressure and fluid shear have all been applied *in situ* in past nanodiffraction experiments at P03, i.e. while high resolution structural information data were recorded. Not only do these results emphasize our focus on materials science but they also demonstrate why X-ray Nanodiffraction is a genuine *in situ* microscopy technique.

MM 26.14 Tue 18:30 Poster B3

An Improved Method for Point Deflection Measurements on Rectangular Membranes — ●BENOIT MERLE¹, KYLE NICHOLSON¹, ERIK HERBERT², and MATHIAS GÖKEN¹ — ¹Materials Science & Engineering 1, Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Erlangen, Germany — ²Materials Science & Engineering, Michigan Technological University, Houghton, USA

The point deflection method has recently emerged as a possible alternative to current micromechanical techniques for measuring the residual stress of thin films. A point deflection experiment consists into deflecting a clamped membrane in its center with a nanoindenter tip. The widespread availability of the required equipment makes the method very promising for future applications. These outlooks were further enhanced by the recent extension of the evaluation theory to rectangular membranes, which - unlike circular ones - are easily fabricated by standard lithographic techniques. In this work, the recent theoretical advances were critically reviewed and an improved experimental method based on the measurement of the contact stiffness was implemented. The new method was applied to the measurement of the residual stress of 100-nm thick SiNx and TiO2 membranes. The accuracy of the point deflection experiments was assessed by testing the same samples a second time with the bulge test reference technique. It is shown that the new experimental method dramatically improves the reproducibility of the measurements, and suggestions are made to improve the current evaluation scheme.

MM 26.15 Tue 18:30 Poster B3

Combining in situ tensile testing and orientation microscopy in the SEM: A MEMS based setup for studying the deformation of thin films — ●JAN PHILIPP LIEBIG, BENOIT MERLE, and MATHIAS GÖKEN — Institute I: General Materials Properties, FAU Erlangen-Nürnberg, Erlangen, Germany

Structures in integrated devices are constantly subjected to residual or thermal stresses during operation. Understanding the relaxation behavior of thin films is therefore critical for improving their reliability. Recently it was shown that Transmission Kikuchi Diffraction (TKD) in the SEM enables the determination of local crystal orientations with high spatial resolution using standard Electron Backscatter Diffraction instrumentation [1]. Giving access to quantitative information on mechanisms like grain growth, grain rotation and strain gradient evolution, time resolved TKD stands out as a promising technique for the characterization of microstructural changes upon relaxation of thin films. We have implemented a MEMS based tensile device [2] into a custom setup specifically designed for in situ TKD imaging inside the SEM. A scanning TEM detector is used complementarily to access shorter time scales. In this context, a novel technique for the preparation and mounting of freestanding thin film tensile samples is presented, which relies on focused ion beam (FIB) milling and selective, electron-beam-assisted etching of silicon membranes.

[1] R.R. Keller, R.H. Geiss, J. Microsc. 245 (2012) 245.

[2] E. Hosseinian, O.N. Pierron, Nanoscale 5 (2013) 12532.

MM 26.16 Tue 18:30 Poster B3

In-operando soft x-ray microspectroscopy of organic field-effect transistors — ●XIAOYAN DU, BENEDIKT RÖSNER, and RAINER FINK — Physikalische Chemie II, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany

Organic semiconducting films bear high potential for organic electronics. While many studies are devoted to the morphology and interface of the semiconducting thin film, investigations of the devices un-

der operation are rather scarce. Microscopic resolution further allows to correlating film morphology with charge transport. Upon application of gate and/or source-drain voltages in organic field-effect transistors (OFETs), the energetic levels of organic semiconductor shift enabling charge accumulation and charge transport. In-operando NEXAFS spectroscopy in Scanning Transmission X-ray Microspectroscopy (STXM) were used to study the density of unoccupied density of states (UDOS). In order to correlate the impact of external fields (gate effect) to energetic shifts of the occupied levels (HOMO, core levels), spatially resolved XPS measurements were explored. In this contribution, we discuss various aspects and limitations of in-operando microspectroscopy using α , ω -dihexyl-sexithiophene (DH6T) based OFETs to obtain full insight into the electronic structure.

MM 26.17 Tue 18:30 Poster B3

Fabrication and application of static liquid cells for transmission electron microscopy — ●ANDREAS HUTZLER¹, ROBERT BRANSCHIED², BENJAMIN BUTZ², MICHAEL P. M. JANK³, LOTHAR FREY^{1,3}, and ERDMANN SPIECKER² — ¹Chair of Electron Devices, FAU Erlangen-Nuremberg, Germany — ²Center for Nanoanalysis and Electron Microscopy, FAU Erlangen-Nuremberg, Germany — ³Fraunhofer Institute for Integrated Systems and Device Technology, Germany

In situ liquid cell transmission electron microscopy (LCTEM) is a highly attractive characterization method for nanoparticle systems, because it enables real time imaging in liquid environment under the high vacuum requirements of electron microscopy. In our approach we present the batch fabrication of custom-designed static liquid cells for conventional specimen holders adapted to the design of Zheng et al. [1]. The basic concept is to confine a fluid in a channel between two electron-transparent membranes enclosed by a silicon frame which is structured by micromachining. Experimentally we could demonstrate growth and degradation processes of Au nano-rods induced by electron beam irradiation. While further development of functionalized cells is ongoing, our aim is the study of various material processes under liquid conditions as well as the enhancement of the LCTEM methodology itself. E.g. radiation damage and resulting secondary effects have not been investigated systematically to date although they have been observed in numerous studies.

[1] H. Zheng et al., Science 2009, **324**, 1309-1312

MM 26.18 Tue 18:30 Poster B3

Electrical Conduction in Thin Layers of ZnO Nanoparticles, Studied Under Various Conditions — ●MOSES RICHTER, JOHANNES C. VOLL, GEBHARD J. MATT, MICHAEL SALVADOR, and CHRISTOPH J. BRABEC — i-MEET, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstraße 7, 91058 Erlangen, Germany

Solution cast thin layers of nanoparticles are important to many novel printed electronics, e.g. organic solar cells, organic LEDs and OFETs. However, stable ink formulations require the use of stabilizing ligands, which strongly influence the electrical conduction in the dried layer, hence the device performance. The limiting conduction mechanism in aforementioned layers is identified in low temperature experiments as a Poole-Frenkel limited transport. By in-situ UV-light treatments under various atmospheric conditions, the responsible defects could be correlated to the particle surfaces. The actual electronic change in UV-light treated ZnO layers is further evaluated by Kelvin Probe-AFM scans and the influence on organic solar cell performance. In latter it turned out to improve the long time stability and maximal achievable performance.

MM 26.19 Tue 18:30 Poster B3

Probing the dynamics of piezoelectric field in GaN nanorods by in-situ bending in transmission electron microscope with differential phase contrast and electron diffraction mapping — ●MINGJIAN WU¹, FLORIAN NIEKIEL¹, CHRISTEL DIEKER¹, SILKE CHRISTIANSEN², and ERDMANN SPIECKER¹ — ¹WW9 & CENEM, Department Werkstoffwissenschaften, FAU Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen, Germany — ²MPI for the Science of Light, Günther-Scharowski-Str. 1, 91058 Erlangen, Germany

Probing the electric properties of functional semiconductors in nanoscale resolution is of great interest, because it allows direct visualization of the relation to the local structure and especially defects. Inversion domain boundary (IDB) is one of the common defects found in wurtzite GaN, a polar crystal with piezoelectricity. As is known, piezoelectricity couples to the polarity of crystal and the sign of applied stresses. For wurtzite GaN nanorods with IDB upon mechanical bend-

ing, the piezoelectric field and charge distribution would be expected to be greatly different to normal GaN nanorods. Experimentally, electric fields can be visualized down to atomic scale, in principle, by the deflection of electron probe (i.e., differential phase contrast (DPC)). In this work, we perform in-situ mechanical bending of GaN nanorods with side-to-side IDB in the TEM, and acquire DPC micrographs and convergent beam electron diffraction pattern arrays to infer the dynamics of piezoelectric field in the GaN nanorods. Interesting findings and comprehensive data evaluation and interpretation will be presented.

MM 26.20 Tue 18:30 Poster B3

Investigating the formation, growth and phase transition of semiconductor nano-crystals in solid by in-situ annealing in TEM — •MINGJIAN WU^{1,2,3}, ESPERANZA LUNA², JANNE PUUSTINEN³, MIRCEA GUINA³, ACHIM TRAMPERT², and ERDMANN SPIECKER¹ — ¹WW9 & CENEM, Department Werkstoffwissenschaften, FAU Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen, Germany — ²Paul-Drude-Institut, Hausvogteiplatz 5-7, 10117 Berlin, Germany — ³Optoelectronics Research Centre, Tampere University of Technology, PO Box 692, 33101, Tampere, Finland

Spontaneous formation of semiconductor nano-crystals in solids is of technological importance and of great scientific interest. It can be driven by the intrinsic tendency to phase separation of metastable compounds, if the atomic diffusion is activated. The controllability of the resulting structure and phase relies on a deeper insight into the atomic diffusion process and defects interaction. This can be scoped by observing individual events and/or from statistics of their time and temperature dependency, which is missing in ex-situ studies. Recently, we observed ex-situ, upon annealing, the formation and phase transformation of Bi-containing nano-crystals embedded in GaAs matrix, which might in principle operate as quantum dots. In this work, we perform in-situ annealing experiments on dedicated Ga(As,Bi) epilayers in the TEM. The dynamics of formation and growth of Bi-containing nano-crystals is revealed; and even their phase transformation and interaction with dislocation loops is observed. We will present the latest results and a comprehensive evaluation and interpretation of the data.

MM 26.21 Tue 18:30 Poster B3

In situ TEM Interfacial Electrochemistry of Fluoride Ion Batteries — MOHAMMED HAMMAD^{1,2}, •MOHAMMAD SALEH GORJI^{1,2}, VENKATA SAI KIRAN CHAKRAVADHANULA^{1,2,3,4}, M. ANJI REDDY^{1,3}, CARINE RONGEAT¹, TORSTEN SCHERER^{1,4}, HORST HAHN^{1,2,3}, MAXIMILIAN FICHTNER^{1,3}, and CHRISTIAN KÜBEL^{1,3,4} — ¹INT, Karlsruhe Institute of Technology (KIT), Germany — ²TU Darmstadt, Germany — ³HIU, KIT, Germany — ⁴KNMF, KIT, Germany

In situ transmission electron spectroscopy provides high spatial resolution visualization of battery operations in real time, giving an important insight on the electrochemistry of batteries. Fluoride ion batteries have a great potential to be an alternative to the conventional Li ion batteries because of the high electronegativity and comparable low atomic weight of the fluorine. In this study, the structural properties of a micron-sized all-solid-state fluoride ion battery at the interfaces between electrolyte and electrodes, and their degradation mechanisms during cycling, have been investigated by in-situ TEM. Ball milling was used to prepare the La_{0.9}Ba_{0.1}F_{2.9} electrolyte and the cathode was a composite of Cu and C and the anode a composite of MgF₂, Mg, La_{0.9}Ba_{0.1}F_{2.9} and C. The battery was cycled between 0 V to 3.5 V. HRTEM micrographs revealed the formation of CuF₂. Additionally, morphological changes observed at the interfaces are presented.

MM 26.22 Tue 18:30 Poster B3

New approach of segmentation of FIB tomograms of porous carbon-rich materials — •MANUEL MUNDZINGER, JÖRG BERNHARD, UTE GOLLA-SCHINDLER, and UTE KAISER — Ulm University, Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Focused ion beam (FIB)-Tomography is widely used in material sciences to gain quantitative information about the topography and composition of the specimen under investigation. With a single tomogram it is possible to determine the volume fraction and the surface of a selected element. Segmentation of FIB tomograms of a porous material can, however, be very troublesome caused by the high depth of focus given by the scanning electron microscope. Thus, the same grey level can be obtained e.g. for the top and the bottom of a pore. This can become the restricting hurdle for a reliable segmentation of the single picture and therefore of the whole tomogram. One possibility is to fill

the pores with resin to decrease the insights in the sample structure. However, many resins are carbon-based and therefore this procedure only works fine as long as the sample does not contain carbon. Here we present a new way to face the problem associated with FIB-tomograms of porous materials with carbon-rich inclusions. For our method we use carbon-free industrial available coatings to avoid the loss of the carbon contrast in the SEM images. The best results were obtained when the sample was hydrophilized using a plasma cleaner, which increased the wetting and therefore the pore filling of the sample greatly.

MM 26.23 Tue 18:30 Poster B3

Towards Conductivity Measurements in Battery Materials Using Scanning Electron Microscopy — •SEBASTIAN STURN, UTE GOLLA-SCHINDLER, JÖRG BERNHARD, and UTE KAISER — Electron Microscopy Group, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

There are several ways of determining the conductivity of bulk materials, especially known in the field of solid state physics. However, the experiments will usually yield only the mean conductivity. We try to spatially resolute the electrical conductivity of state-of-the-art secondary battery electrodes by means of injecting electrons using an SEM.

In a first step, it is necessary to determine the amount of incident electrons absorbed in the bulk material. It is therefore crucial to quantitatively characterize any electron current exiting the specimen, namely the secondary electron and backscattered electron current, since the absorbed current is given by $I_{abs} = I_{incident} - I_{SE} - I_{BSE}$.

The approach is to directly measure I_{SE} and I_{BSE} for every spot of the scan pattern. By using Focused Ion Beam (FIB), we are able to get rid of the specimen's topography and prepare polished surfaces. As the secondary electron yield is mainly dependent on the topography, we are able to, at least as a first approximation, assume that the secondary electron current is constant.

The use of a Gas Injection System (GIS) allows for sputtering platinum contacts on top of the specimens. We use these platinum pads as contact areas for micromanipulators to read out absorbed currents.

MM 26.24 Tue 18:30 Poster B3

Interaction of hydrodynamic cavitation bubbles with textile linen in an open reactor — PATRICK CASPER, TAMARA NEUMANN-SCHMIDT, •FLORIAN SZILLAT, HANS-GÜNTER HLOCH, and JÜRGEN BOHNEN — wfk - Cleaning Technology Institute, D-47807 Krefeld, Deutschland

The amount of individually and fashionably Corporate Identity clothing is increasing in hygienically demanding areas. During reprocessing of such clothing, extensive hygiene measures have to be fulfilled. Meeting high demands on non-destructive textile processing and sustainability as well as hygiene requirements, the use of hydrodynamic cavitation is of great interest, as it is providing mechanical impact and reactive oxygen species under textile preserving conditions. Recent studies (e.g. [1]) demonstrated the capability of hydrodynamic cavitation in the field of pharmaceuticals/chemicals degradation. These systems are based on venturi nozzle or orifice plate design in closed tubular systems, whereas an open environment is necessary for reprocessing of clothing. To obtain a better understanding of behaviour of hydrodynamic cavitation bubbles outside of nozzles and such tubular systems their distribution in an open reactor is studied using luminescence. Furthermore, interplay of parameters and nozzle design is investigated by means of dye destruction analysis. Implications of bleaching and disinfection as well as influence of design and parameters on the use of hydrodynamic cavitation at water-textile interfaces will be discussed.

[1] P. Braeutigam et al. Water Research 46 (2012) 2469

MM 26.25 Tue 18:30 Poster B3

Mechanical properties of 3D printed polymers on textile fabrics with interface layer modification — •NILS GRIMMELSMANN¹, MIRJA LUTZ², MICHAEL KORGER², HUBERT MEISSNER¹, and ANDREA EHRMANN¹ — ¹Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld, Germany — ²Niederrhein University of Applied Sciences, Mönchengladbach, Germany

Composites produced from two or more different materials with different physical and chemical properties often allow for tailoring mechanical and other characteristics of the resulting multi-material system. Fiber-reinforced plastic composites have usually high strength and elasticity due to a combination of the tough but weak plastic ma-

trix with the strong and stiff reinforcing fibers, filaments or textile layers.

Combinations of textile materials with 3D printed polymers, however, result in different mechanical properties of the composites. While the tensile strength of the multi-material system is increased compared to the pure 3D printed material, the elasticity of the polymer layer can be retained to a certain degree, since the textile material is not completely immersed in the polymer. Instead an interface layer is built in which both materials interpenetrate to a certain degree.

The poster will give an overview of the parameters affecting the interface layer. The influence of this interface layer on possible delamination and mechanical properties of the developed composites will be depicted, resulting in the possibility to tailor the desired strength and elasticity of polymer-textile composites.

MM 26.26 Tue 18:30 Poster B3

Synthesis and electrochemical properties of orthorhombic α -MoO₃ and hexagonal h-MoO₃ nanostructures — ●CHRISTINA SCHMIDT¹, ALEXANDER OTTMANN¹, GALINA ZAKHAROVA², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute for Physics, University of Heidelberg, Germany — ²Institute of Solid State Chemistry, Ural Division, Russian Academy of Sciences, Yekaterinburg, Russia

MoO₃ nanomaterials with either hexagonal or orthorhombic crystal structure have been synthesised by means of a microwave-assisted hydrothermal route. The different structures are obtained by varying the synthesis parameters, which also leads to different size and shape of the primary particles. Magnetisation studies by means of SQUID magnetometry allow assessing that less than 0.1% of Mo⁵⁺-defects are present in the materials. The electrochemical properties of the different samples are studied by means of cyclic voltammetry and galvanostatic cycling, and are discussed with regard to the XRD, SEM and SQUID data. Cyclic voltammetry reveals reversible processes associated with the Mo⁶⁺/Mo⁵⁺ redox couple in the α -MoO₃ nanostructures. Galvanostatic cycling within the potential limits of 1.5-3.5 V vs. Li/Li⁺ of α -MoO₃ nanorods shows an initial discharge capacity of 296 mA h g⁻¹ at 100 mA g⁻¹. In case of h-MoO₃ nanostructures, except for large irreversible initial effects, only low electrochemical activity is observed.

MM 26.27 Tue 18:30 Poster B3

Doping studies and structural, magnetic, and electrochemical characterization of tetrahedral LiCo_{1-x}M_xPO₄ (M = Cu, Fe, Zn, Y) — ●YUQUAN WU¹, VERENA NEDER¹, BENJAMIN HERDEANU¹, LUCAS SCHLESTEIN¹, HANS-PETER MEYER², CHRISTOPH NEEF¹, and RÜDIGER KLINGELER¹ — ¹Kirchhoff-Institute for Physics, Heidelberg University, Heidelberg, Germany — ²Institut für Geowissenschaften, Heidelberg University, D-69120 Heidelberg, Germany

Tetrahedral LiCo_{1-x}M_xPO₄ microstructures with transition metals M such as Cu, Fe, Zn, and Y are synthesized by a microwave-assisted hydrothermal method. For each dopant, the accessible doping range x is studied and the effect of doping on the crystal structure as well as on the morphology is investigated. Non-magnetic Zn-doping allows investigating the slightly diluted magnetic system LiCo_{1-x}Zn_xPO₄ with x 0.05, as well as paramagnetic LiCo_{0.05}Zn_{0.95}PO₄ which enables studying well separated magnetic Co-centers. Regarding the electrochemical behavior, low doping levels enhance the intercalation kinetics while high doping levels yield a clear reduction of electrochemical capacity as demonstrated by cyclic voltammetry. In contrast to well known olivine-like LiFePO₄, the iron doped tetrahedral structure shows no appreciable electrochemical activity that can be clearly associated with the Fe²⁺/Fe³⁺ redox couple.

MM 26.28 Tue 18:30 Poster B3

Hydrogen treatment of Fe₆₀Al₄₀ thin films — ●JONATHAN EHRLER^{1,2}, RANTEJ BALI¹, CAMILO OTALORA¹, WOLFGANG ANWAND¹, ROMAN BÖTTGER¹, MACIEJ O. LIEDKE¹, THOMAS G. WOODCOCK³, and KAY POTZGER¹ — ¹HZDR, Bautzner Landstrasse 400, 01328 Dresden, Germany — ²Dresden University of Technology, Helmholtzstrasse 10, 01069 Dresden, Germany — ³IFW Dresden, PO Box 270116, 01171 Dresden, Germany

The effect of H treatment on the magnetic properties and the defect concentration of Fe₆₀Al₄₀ films, possessing A2 and B2 structure respectively, have been investigated. The treatment was realized by H⁺ irradiation as well as by reactor loading. Ferromagnetic A2-Fe₆₀Al₄₀ films of 250 nm thickness were irradiated with protons at an energy of 17 keV and fluences of up to 1.46 E18 ions cm⁻². Magneto-optical Kerr effect showed a variation of coercivity and an increase of saturation magnetization (M_S) as a function of ion fluence. Positron annihilation spec-

trosopy (PAS) indicates an increase of the open volume defect concentration. Superparamagnetic B2-Fe₆₀Al₄₀ films were annealed at 423 K in 30 bar H atmosphere. PAS shows that the H-annealing process led to a decrease in the open volume defect concentration. H-treatment caused a small increase in M_S from 0.013 to 0.017 μ_B /Fe atom, as well as a shift in the blocking temperature from 85 to 115 K respectively. While H treatment significantly modifies the magnetic properties of Fe₆₀Al₄₀, elastic recoil detection suggests that the hydrogen is not retained in the vacancies present in the film, suggesting that the variations may be mostly due to structural changes.

MM 26.29 Tue 18:30 Poster B3

Mg₂Fe(x)Si(1-x) - hydride: The interplay between, defects, structure and magnetic properties — ●THU TRANG TRINH^{1,2}, OGUZ YILDIRIM¹, OSKAR LIEDKE¹, WOLFGANG ANWAND¹, ANDREAS WAGNER¹, KOHTA ASANO³, BERNARD DAM⁴, and KAY POTZGER¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — ²Dresden University of Technology, Helmholtzstrasse 10, 01069 Dresden, Germany — ³Energy Technology Research Institute, Ibaraki 305-8565, Japan — ⁴Delft University of Technology, 2628 BL Delft, Netherlands

Mg₂Fe hydride belongs to the most promising candidates for application as light weight storage material in a future hydrogen economy. Recently, it has also been shown that due to chemochromism, Mg₂Fe is a low-cost and rare-earth-free candidate for switchable mirrors upon hydrogen loading. Besides the Mg₂Fe hydride, a new compound of Mg₂(FeSi) will be presented. The additional content of Si promises an optimization of hydrogen absorption and desorption processes. The Fe component of the system makes it an interesting material in terms of magnetic applications. Comprehensive investigations on Mg₂(FeSi) system showed that hydrogen induced changes in structure, electronic, optical and magnetic properties. E.g., volume magnetic properties transform from superparamagnetism to ferromagnetism with a high Curie temperature. In order to understand the basic physical properties of Mg₂(FeSi) thin films and its hydride the present studies involve fundamental research and defect analysis.

MM 26.30 Tue 18:30 Poster B3

Thermal decomposition of sodium borohydride covered with polyethyleneimine — ●HENDRIK RAHMANN¹, CHRISTIAN STERNEMANN¹, SEBASTIAN DAHLE², GEORGIA SOURKOUNI², CHRISTOS ARGIRUSIS^{2,3}, KARIN ESCH¹, FLORIAN WIRKERT¹, HOLGER GÖHRING¹, WOLFGANG MAUS-FRIEDRICHS², and METIN TOLAN¹ — ¹Technische Dortmund, 44221 Dortmund, Germany — ²Technische Universität Clausthal, 38678 Clausthal-Zellerfeld, Germany — ³National Technical University of Athens, 15773 Zografou/Athens, Greece

In order to use hydrogen as an energy carrier in the future as part of real-life technologies, efficient hydrogen storage media are necessary. Borohydrides are an attractive hydrogen storage material because of their low mass and high hydrogen density. Here, one of the promising candidates is sodium borohydride (NaBH₄) if its degradation at atmosphere can be hindered and its hydrogen release temperature can be lowered. To achieve this goal, NaBH₄ can be covered with a polyethyleneimine (PEI) layer [1]. We performed in situ X-ray diffraction (XRD) measurements at beamline BL9 of DELTA synchrotron radiation source using native and PEI-coated NaBH₄ while heating the samples from 30°C to 720°C. The crystalline reaction products at different temperatures were determined in order to compare both hydrogen release paths. Moreover we applied quadrupole mass spectrometry and differential scanning calorimetry to characterize changes in the hydrogen desorption path of NaBH₄ induced by PEI coverage.

[1] S. Dahle et al., RSC Adv. 4, 2628 (2014).

MM 26.31 Tue 18:30 Poster B3

Materials for all solid-state thin-film batteries — ●SUSANN NOWAK¹, PRIYANKA SHARMA¹, GIULIO CALCAGNO¹, MATTHIAS KÖHLER², JULIANE MÜRTER¹, FABIAN WUNDE², and GUIDO SCHMITZ¹ — ¹Heisenbergstr. 3, 70569 Stuttgart — ²Wilhelm-Klemm-Str. 10, 48149 Münster

All solid-state batteries received increasing attention over the last years due to the simplified packaging process and increased energy density and safety. The defined thin-film geometry is also well suited to conduct fundamental studies of thermodynamics and kinetics of batteries. Since batteries are complex multilayer devices, it is essential to optimize and characterize anode, cathode and electrolyte materials carefully before combining them in an all solid-state battery. This contri-

bution presents a wide construction-kit of different battery materials which can be successfully produced by ion-beam sputtering. In particular the fabrication and properties of LFP, LMO, LCO, NMC, Sn, Si and LiPON as thin films are shown. Challenges of balancing a full cell and its effects on the energy density of a battery are discussed on a LFP-Sn anode-cathode model. First results on combining battery materials are shown. The behavior of the storage materials can vary drastically due to differing interfacial properties.

MM 26.32 Tue 18:30 Poster B3

Deposition of transition metal oxide thin film cathode materials for Li-ion battery application — ●GEOFFREY MATTHEW TAN¹, CHRISTOPH LOHO¹, OLIVER CLEMENS^{1,2}, and HORST HAHN^{1,2,3} — ¹Joint Research Laboratory Nanomaterials, Darmstadt, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — ³Helmholtz Institute Ulm, Ulm, Germany

The development of smaller and more powerful electronic devices places a strong demand on energy sources that are compact, safe and have a high energy density. Solid state thin film lithium ion batteries are one of the candidates to fulfill this demand. The use of aerosol assisted chemical vapor deposition (AA-CVD) to precisely control stoichiometry in nickel substituted LiCoO₂, which acts as cathode in such a device, is a possible strategy to increase the energy density.

The aim of this study was to find the optimum process parameters for LiCoO₂ thin film deposition using AA-CVD and to substitute cobalt by nickel to form lithium nickel cobalt oxide, because of its higher energy density and lower cost.

The structure, morphology and phase composition of LiCoO₂ films as well as nickel substituted films were studied comprehensively. Phase pure LiCoO₂ was deposited at 850 °C. Electrochemical characterization in a Swagelok type half-cell demonstrated a specific capacity of 94 mAh/g for LiCoO₂. Despite the precise control of the nickel to cobalt ratio, the deposited thin films do not show the desired phase. Their electrochemical activity will be discussed.

MM 26.33 Tue 18:30 Poster B3

Surface Excess Elasticity: A First-Principles Study — ●BEATRIX ELSNER and STEFAN MÜLLER — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 HH

The size-dependent elastic response of nanomaterials and nanostructures with a large surface-to-volume ratio has attracted increasing attention. Yet, it remains an open question whether the presence of surfaces entails a stiffening or softening of the material [1]. The surface elastic constants—a measure for the change of surface stress with surface strain—represent a key quantity with regard to this question. In this contribution, we present a density functional theory (DFT) study of the surface energy, surface stress, and surface elastic constants of low-index fcc metal surfaces. Our calculations yield positive surface elastic constants for the (111) and (001) surfaces of gold, implying a stiffening effect.

Supported by DFG, SFB 986, project B3.

[1] Mameka, et al., *Acta Materialia* **76**, 272 (2014).

MM 26.34 Tue 18:30 Poster B3

Quantum mechanically based prediction of surface segregation in Ag-Au alloys — ●SANDRA HOPPE and STEFAN MÜLLER — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (npAu) offers a high catalytic activity for certain chemical reactions combined with a high selectivity. This phenomenon can theoretically be explained in two ways: First, the rough morphology provides a large number of low-coordinated Au atoms. Second, Ag impurities remaining from the dealloying process may supply reaction sites. Interestingly, Au (111) surfaces roughened by sputtering have been found inactive towards CO-oxidation [1]. Previous density functional theory (DFT) results imply that Ag impurities in the surface dissociate molecular O₂ and supply O atoms [2]. Experimental results show that the catalytic activity of npAu can be tailored via the residual Ag concentration. The aim of this work is to characterize clean Ag-Au surfaces regarding their segregation profile. DFT calculations serve as input for a surface cluster expansion (CE). We find that the resulting surface composition depends strongly on the applied exchange correlation functional. To obtain Ag enrichment in the surface layer, as it has been observed in experimental and theoretical studies [3], it seems necessary that both the lattice parameters and the surface energies of

the pure elements are calculated in the correct hierarchy.

[1] J. Gong *et al.*, *J. Phys. Chem. C* **112** (2008) 5501.

[2] L. V. Moskaleva *et al.*, *Phys. Chem. Chem. Phys.* **13** (2011) 4529.

[3] e.g. T. Déronzier *et al.*, *J. Catal.* **311** (2014) 221.

MM 26.35 Tue 18:30 Poster B3

The formation of nc-Si in SiOx induced by continuous-wave laser irradiation — ●NAN WANG¹, THOMAS FRICKE-BEGEMANN², PATRICK PERETZKI¹, MICHAEL SEIBT¹, and JÜRGEN IHLEMANN² — ¹IV. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²Laser-Laboratorium Göttingen, Hans-Adolf-Krebs-Weg 1, 37077 Göttingen, Germany

Silicon nanocrystals embedded in substoichiometric SiO_x (silicon-rich silicon oxide) exhibit room-temperature photoluminescence due to quantum confinements. The generation of nc-Si can be induced by thermal annealing or laser irradiation. It is known that laser irradiation on free-standing SiO_x without substrate may avoid the heat flow into the substrate. Here we employ continuous-wave laser irradiation at 405 nm wavelength to focus a 6 μm diameter spot on 545 nm thick SiO_x films deposited on fused silica substrates. A high density of nc-Si particles is obtained. The samples are characterized by AFM, TEM, Raman spectroscopy and photoluminescence. The spatial distribution of the nanocrystals in the irradiated area is determined. At a laser irradiance of 1.2·10⁵ W/cm², an almost perfect damage-free irradiation is obtained. At higher laser power the central region exhibits some porous properties, and the nc-Si region is located beneath the porous region. In summary, we have demonstrated that laser annealing offers the possibility to generate Si nanoparticles in a fast, high throughput process. Also, the thermal load on the substrate can be significantly reduced.

MM 26.36 Tue 18:30 Poster B3

Synthesis and characterization of bulk heterojunction solar cells based on nanoporous templates — ●SVEN HILKE¹, YONGGANG ZHEN², WENPING HU², and GERHARD WILDE¹ — ¹Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Institute of Chemistry, Chinese Academy of Sciences, ZhongGuanCun North First St 2, Beijing 100190, P. R. China

The well-known system Zn-Phthalocyanine:Fullerene (ZnPc:C60) as a model system of bulk-heterojunction solar cells has been chosen to analyze the effect of a nanoporous structuring on the applicability of the resulting hetero molecular mixture. In this context, the basis of the pre-structuring is an Anodic Aluminum Oxide (AAO) membrane made of aluminum oxide constructed by electrochemical processes. The controlled wet-chemical deposition via the dipNdry (dipping and drying) method generates tubes or rods (depending on concentration, solvent as well as dipping time and repetition). Naturally, the pre-structuring directly influences the morphology on the nanometer scale. The presented work consists of the controlled growth of the nanoporous templates to obtain regular pore structures with equal and uniformly distributed surface area in the hetero intersection. In addition, every single nanopore is individually functional so that the failure of a single nanopore does not cause the destruction of the whole solar cell. Scanning electron and scanning tunneling microscopy, as well as optical characterizations are used to analyze the obtained structures.

MM 26.37 Tue 18:30 Poster B3

Computational design of metal-organic frameworks with paddlewheel-type secondary building units — ●UDO SCHWINGENSCHÖGL, MAXIM V. PESKOV, and NEJIB MASGHOUNI — PSE Division, KAUST, Thuwal 23955, Saudi Arabia

We employ the TOPOS package to study 697 coordination polymers containing paddlewheel-type secondary building units. The underlying nets are analyzed and 3 novel nets are chosen as potential topologies for paddlewheel-type metal organic frameworks (MOFs). Dicarboxylate linkers are used to build basic structures for novel isorecticular MOF series, aiming at relatively compact structures with a low number of atoms per unit cell. The structures are optimized using density functional theory. Afterwards the Grand Canonical Monte Carlo approach is employed to generate adsorption isotherms for CO₂, CO, and CH₄ molecules. We utilize the universal forcefield for simulating the interaction between the molecules and hosting MOF. The diffusion behavior of the molecules inside the MOFs is analyzed by molecular dynamics simulations.

MM 26.38 Tue 18:30 Poster B3

A new method for synthesis of graphite oxide nanoplatelets

from bamboo pyrolytic acid: Morphological, structural and transport properties — ●KATHERINE GROSS¹, JHON J. PRIAS^{2,3}, SORAYA SANGIAO⁴, JOSE M. DETERESA⁴, HERNANDO ARIZA², and PEDRO PRIETO¹ — ¹CENM, Universidad del Valle, Colombia — ²IIS, Universidad del Quindío, Colombia — ³EITP, Universidad del Quindío, Colombia — ⁴LMA, INA Universidad de Zaragoza, Spain

In this work we present a new and cost-effective method for the synthesis of graphite oxide nanoplatelets (GONP) using bamboo pyrolytic acid (BPA) as source. Characterization by Raman, FTIR and XRD techniques confirm that increased carbonization temperature increases graphite conversion. GONP-BPA present lateral dimensions of $5\text{-}100 \times 10^3$ nm and thickness less than 80 nm. HRTEM and EEL spectra reveal that locally the carbon is mainly in sp² bonding configuration and confirm a short/medium range of crystalline order. For electrical characterization, single nanoplatelets were contacted by focused-ion-beam-induced deposition of Pt nanowires. The electrical conductivity at room temperature shows a rise of three orders of magnitude by reducing the atomic percentage of oxygen from 17 to 5 percent, reaching a final value of 2.3×10^3 S/m. Temperature-dependent conductivity measurements show a semiconductor-like behavior with weak temperature dependence. This research shows that BPA can be used for sustainable creation of graphitic carbon which could be used in the development of advanced devices.

MM 26.39 Tue 18:30 Poster B3

Comparison of nanoparticles in printer toners between original equipment manufacturer to office supplies manufacturer — ●PAULA WEBER, MIRIAM LEIFELS, and MATHIAS GETZLAFF — Heinrich-Heine-Universität Düsseldorf

We use laser printer toners in our everyday life. To identify its composition and the material properties we must examine it at the nanoscale. So we can, for example, observe a lot of different nanoparticles in printer toners. The differences between the various printer toner manufacturers in terms of nanoparticles relating to the size, the element composition as well as the various physical properties are remarkably.

This contribution will exemplarily discuss the comparison between the printer toner of original equipment manufacturer and the printer toner of office supplies manufacturer.

Different experimental techniques make the comparison possible. These include Dynamic Light Scattering (DLS), X-Ray Diffraction (XRD), Transmission Electron Microscope (TEM), Scanning Electron Microscope (SEM) and Energy Dispersive X-Ray Spectroscopy (EDX).

The sizes can be measured by DLS and electron microscopy. XRD allows to obtain information on the structure of the nanoparticles. The remaining questions can be answered by a specific SEM with integrated EDX.

By comparing the results of the various above mentioned methods, we get knowledge concerning the used nanoparticles.

Finally, the nanoparticles of the two different manufacturers are compared with each other to determine the similarities and differences.

MM 26.40 Tue 18:30 Poster B3

Oxygen vacancy diffusion in sodium bismuth titanate studied by density functional theory calculations — ●KAI-CHRISTIAN MEYER, MELANIE GRÖTING, and KARSTEN ALBE — TU Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

Sodium bismuth titanate ($\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$, NBT) is a ferroelectric relaxor-like material at room temperature and has interesting electrical properties for application as a high strain actuator material. It shows a broad diffuse phase transition from a ferroelectric (rhombohedral/monoclinic) structure to a weakly polar (tetragonal) state. Recently, it has been shown that doped NBT exhibits a high ion conductivity, in contrast to other perovskites. [1] Thus, in this work we investigate by means of density functional theory calculations oxygen vacancy formation energies, association energies with different metal ions and migration barriers for different A-cation orders. We find among other things that the chemical order plays a strong role on the atomistic level, eg. for local phase transitions [2] and conductivity.

[1] M. Li, *et al.*, Nat. Mater. 13, 31 - 36 (2014)

[2] K.-C. Meyer, *et al.*, J. Solid State Chem. 227, 117 - 122 (2015)

MM 26.41 Tue 18:30 Poster B3

Nonequilibrium Dynamics of the spin system and lattice heat in the rare earth Dysprosium — ●ALEXANDER VON REPPERT¹, JAN PUDELL¹, KARINE DUMESNIL², FLAVIO ZAMONI¹, and MATIAS BARGHEER^{1,3} — ¹Institut für Physik und Astronomie, Potsdam, Germany — ²Institut Jean Lamour, Vandoeuvre les Nancy cédex, France — ³Helmholtz Zentrum Berlin, Berlin, Germany

We present a temperature and fluence dependent Ultrafast X-Ray Diffraction study of a laser-heated Dysprosium thin film. A pronounced lattice contraction heralds the ultrafast loss of antiferromagnetic order, which is reestablished on a nanosecond timescale when the heat reservoir of the phonons in Dy has cooled well below the Néel temperature. The calibration of the position and width of the Bragg peaks in thermal equilibrium allows for a detailed experimental measurement of the energy deposited in the lattice and spin system. Reestablishing the magnetic order by cooling of the magnetic system is much slower than cooling the lattice, especially around the Néel temperature. Although the system shows very strong magnetostriction, the transfer of energy from the spin system to the lattice is weak after the spin-order is lost.

MM 26.42 Tue 18:30 Poster B3

In situ microscopy of material transport and Ge crystallization in the Al-induced layer exchange (ALILE) process — ●JANIS WIRTH, SIMON M. KRASCHEWSKI, and ERDMANN SPIECKER — Lehrstuhl für Mikro- und Nanostrukturforschung und Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg, Erlangen, Germany

The Al-induced layer exchange (ALILE) process exploits the phenomenon of metal-induced crystallization to fabricate polycrystalline seed layers of Si or Ge at low temperatures [1, 2]. In order to understand the process and the material transport involved we use a combination of different in situ microscopy techniques. At low magnification in situ light microscopy reveals the nucleation and growth of crystalline nuclei as well as the overall kinetics of the process. At higher magnification in situ STEM is employed for studying the details of material transport at and near the crystallization front. Due to the small difference in atomic numbers of Al and Si, the Si-ALILE process cannot be directly visualized by Z-contrast imaging. Using Ge instead of Si, Z-contrast imaging benefits from the considerably larger difference in the atomic number. Similar to Si-ALILE, the Ge-ALILE process is characterized by a layer exchange using a stack of a-Ge/ AlO_x /Al on glass or SiN_x substrate at temperatures of 220-417°C. Ge diffuses into the Al layer and forms crystalline precipitates upon supersaturation. Subsequently the precipitates grow while the Al is pushed up into the a-Ge top layer.

[1] J. Schneider et al., J. Non-Cryst. Solids 352, (2006)

[2] K. Nakazawa et al., J. Solid State Science 2 (2013)

MM 26.43 Tue 18:30 Poster B3

Local measurement of stress-strain-curves by spherical nanoindentation — ●PATRICK S. FELDNER, BENOIT MERLE, and MATHIAS GÖKEN — Materials Science and Engineering 1, Friedrich-Alexander-University Erlangen-Nürnberg (FAU)

In contrast to sharp indenters, spherical indenters offer the possibility to determine continuously the stress-strain response of a material at a very local scale. However due to the complex deformation field, various approaches are available for approximating the stress and strain during spherical nanoindentation experiments, leading to significantly different evaluations of the yield behavior of the material.

The aim of this work was to establish a reliable analysis procedure to turn nanoindentation raw data into meaningful stress-strain-curves. This procedure was further extended to the development of a new method for determining the strain-rate sensitivity of flow stress as a function of strain. In the case of ultrafine-grained metallic materials, it is shown that this information in combination with other micromechanical and structural characterization methods, could give new insights into the evolution of the different deformation mechanisms in dependence of the imposed strain.

MM 27: Invited talk Rösner

Time: Wednesday 9:30–10:00

Location: H38

Invited Talk

MM 27.1 Wed 9:30 H38

The secret of shear bands — ●HARALD RÖSNER — WWU Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

Plasticity of metallic glasses is generally still puzzling since in contrast to crystalline materials no comparable deformation carriers such as dislocations, twins or grain boundaries exist. Deformation tests on metallic glasses performed well below the glass transition temperature have shown that the plastic flow is restricted to narrow regions called shear bands. The current understanding is that dilated zones of increased excess volume caused by shear localization enable shear softening. In my talk I will introduce a new method for quantitative density measurements in amorphous materials combining several quantitative

electron scattering signals [1,2]. Density measurements in shear bands of different metallic glasses ($\text{Al}_{88}\text{Y}_7\text{Fe}_5$, $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$, Vitreloy-105) show a unique propagation behavior; that is, alternating high and low density regions. Similar behavior has been reported for granular media, but not for amorphous solids. One important implication is that individual shear bands apparently propagate via local, segment-wise stick-slip that might originate from their complex topology. These results suggest connections to the physics of granular materials and jammed systems.

[1] H. Rösner, M. Peterlechner, C. Kübel, V. Schmidt, and G. Wilde, *Ultramicroscopy* 142 (2014) 1-9.

[2] V. Schmidt, H. Rösner, P.M. Voyles, M. Peterlechner, G. Wilde, *Physical Review Letters* 115 (2015) 035501.

MM 28: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science II - Atomic structure and defects I

Time: Wednesday 10:15–11:45

Location: H38

Topical Talk

MM 28.1 Wed 10:15 H38

In-situ diffraction during complex — ●STEVEN VAN PETEGEM¹, AINARA IRASTORZA^{1,2}, ANTOINE GUITTON¹, MANAS UPADHYAY¹, TOBIAS PANZNER¹, DANIEL GROLIMUND¹, ANTONIO CERVELLINO¹, and HELENA VAN SWYGENHOVEN^{1,2} — ¹Paul Scherrer Institut, CH-5232 Villigen, Switzerland — ²École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

A major challenge in metallurgy is to understand the relation between the microstructure of a metal and its behaviour under an applied load or temperature. This requires a detailed characterization of the evolution of the microstructure at different length scales through the determination of the crystal structure, defect density, grain size distribution, texture etc. During last decade in-situ mechanical testing at the synchrotron/neutron source has become a widespread tool to investigate the evolution of the microstructure of single and polycrystals during deformation. Many such in-situ deformation tests are performed during continuous or interrupted uniaxial tensile and/or compression tests. While such tests have proven to be very useful, for further refinement of crystal plasticity models it is crucial to perform in-situ experiments while changing the strain path. In this work we highlight two such experiments i) in-situ cyclic shear of Cu single crystals, where the formation of a channel-vein structure can be tracked and visualized and ii) in-situ x-ray and neutron diffraction during multiaxial testing.

MM 28.2 Wed 10:45 H38

In situ investigation of the microstructure in friction stir welded steels using high-energy X-ray diffraction — ●MALTE BLANKENBURG, PETER STARON, TORBEN FISCHER, NORBERT SCHELL, LUCIANO BERGMANN, JORGE F. DOS SANTOS, NORBERT HUBER, ANDREAS SCHREYER, and MARTIN MÜLLER — Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Max-Planck-Straße 1, 21502 Geesthacht, Germany

Thermo-mechanical treatments of engineering metallic materials yield non-equilibrium microstructures, which potentially reduce strength and toughness of a joint. As a solid state joining process, friction stir welding reduces the heat input and increases the mechanical properties of the weld. The intermediate stages of phase transformations in the weld zone *during* the joining process can only be studied by *in situ* experiments. Therefore, *in situ* diffraction measurements using a transportable friction stir welding system (FlexiStir) were performed at the HZG high-energy material science beamline (HEMS) at DESY. Due to the high brilliance of the source and a fast PerkinElmer area detector, the investigation of the ferrite and austenite content of a small gauge volume (0.5mm^3) with image rates up to 10Hz was possible. Two different steels (S355, 1.4410) were welded using different welding parameters. The results of the Rietveld refinement deliver a spatially resolved insight to the phase transformations taking place in a short distance behind the welding tool ($<10\text{mm}$) and show a correlation to the welding power.

MM 28.3 Wed 11:00 H38

Single-shot full strain tensor and texture determination of micron-sized samples with white x-ray microbeams — ●ALI ABOUD¹, CHRISTOPH KIRCHLECHNER², TUBA CONKA-NURDAN³, LOTHAR STREUDER⁴, and ULLRICH PIETSCH¹ — ¹University of Siegen, Siegen, Germany — ²Max-Planck-Institut für Eisenforschung, Dusseldorf, Germany — ³Türkisch-Deutsche Universität, Istanbul, Turkey — ⁴PNSensor GmbH, München, Germany

Conventional three dimensional structure determination and the characterization of strain states in a single crystal require either a series of measurements at different orientations or the use of a tunable X-ray source. Here we report on the experimental procedure to determine structure and strain tensor by single shot exposure on micron level using focused white synchrotron radiation. X-ray diffraction Laue patterns are collected from a micro-sized Copper pillar along the bending axis using focused synchrotron radiation. Taking advantage of an energy dispersive 2D camera (pnCCD) we reconstructed the 3D structure of the crystal at each step. At the same time, both the deviatoric and hydrostatic parts of the strain tensor were determined. As an outlook, we show an extension of the developed procedure to be applied in the study of inter- and intra- granular interactions in polycrystalline Nickel samples.

MM 28.4 Wed 11:15 H38

Microstructural Evolution in severely deformed Cu-Ni alloys — ●FRIEDERIKE EMEIS, YULIA BURANOVA, VITALIJ SCHMIDT, JÖRN LEUTHOLD, HARALD RÖSNER, and GERHARD WILDE — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, D-48149

The microstructure evolution of Cu-Ni alloys with different compositions was investigated after severe plastic deformation using high pressure torsion (HPT) with different number of turns followed by annealing. The microstructure evolution is influenced by the stacking fault energy (SFE), which indicates how easily dislocations can form and, therefore, how likely a material is to undergo twinning. The SFEs of the different compositions were experimentally determined by the dissociation width of the present dislocation using high resolution transmission electron microscopy. Twin grain boundaries and especially their conjunction to $\Sigma 3$ - $\Sigma 3$ - $\Sigma 9$ -triple junctions are expected to give more thermal stability to materials. The presence of twins (especially nano-scale twins) was analyzed and grain boundary distributions, grain size distributions and hardness were characterized using electron backscatter diffraction (EBSD), TEM and Vickers Hardness measurements. The obtained results are discussed concerning the impact of the SFE on microstructure evolution during severe plastic deformation.

15 min. coffee break

MM 29: Topical session: Caloric effects in ferroic materials III - Electrocalorics

Time: Wednesday 10:15–11:45

Location: H39

MM 29.1 Wed 10:15 H39

Abnormal electrocaloric effect studied by lattice based Monte-Carlo simulations — ●KAI-CHRISTIAN MEYER, CONSTANZE KALCHER, ALEXANDER STUKOWSKI, and KARSTEN ALBE — TU Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

The abnormal electrocaloric effect (ECE) was first found by Peräntie *et al.* in 2010 in PMN-PT single crystals. [1] Contrary to the normal ECE, an increase of the electric field leads in these materials to a decrease of the temperature. In this work we show that the abnormal ECE can be described within a lattice based random bond model that only includes next neighbor interactions and an external electric field. The negative temperature change can be observed when the electric field lowers the order (configurational entropy) of the polarization vectors. This is the case when the system is in a antiferroelectric state or polar defects with polarization antiparallel to the external field are present. These findings are in agreement with a more elaborate model which includes long-range dipole-dipole interaction and gradient terms. [2]

[1] J. Peräntie, *et al.*, Phys. Rev. B 82, 134119 (2010)

[2] Y. Ma, *et al.*, arXiv:1507.05004

MM 29.2 Wed 10:30 H39

Role of polarization anisotropy in epitaxial PMN-PT thin films for electrocaloric studies — ●MICHAEL MIETSCHKE^{1,2}, O. MEY^{1,2}, C. MOLIN³, S. GEBHARDT³, P. CHEKONIN¹, S. FÄHLER¹, K. NIELSCH¹, L. SCHULTZ¹, and R. HÜHNE¹ — ¹IFW Dresden — ²TU Dresden — ³Fraunhofer IKTS Dresden

A prominent example for electrocaloric (EC) materials are $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$ (PMN-PT) compounds, which are typically used for high performance actuator applications due to its outstanding piezoelectric properties. As the structural and functional properties of these materials are well-known they might serve as a suitable model system to study the interplay between microstructure and EC properties. Since ferroic materials exhibit a strong anisotropy, we will probe the role of polarization anisotropy on the ECE by variation of the film orientation. Epitaxial films are a useful tool to analyze this correlation in order to optimize the performance of these materials.

Therefore, epitaxial 0.9PMN-0.1PT films were grown by pulsed laser deposition on (001)-oriented and (111)-oriented SrTiO_3 single crystalline substrates using an epitaxial $\text{La}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$ buffer as bottom electrode and additional Au top electrodes. The structural properties were studied by high resolution XRD, AFM and TEM. The anisotropy of the ferroelectric domain structure was investigated by vertical and lateral piezoresponse force microscopy. The indirect determination of the EC properties was performed by temperature dependent polarization measurements at different electric fields. Funded by SPP 1599.

MM 29.3 Wed 10:45 H39

Electric field direction dependence of the electrocaloric effect in BaTiO_3 : a first principles effective Hamiltonian approach — ●MADHURA MARATHE¹, DAMIAN RENGGLI¹, ANNA GRÜNEBOHM², and CLAUDE EDERER¹ — ¹Materials Theory, ETH Zürich, Switzerland — ²Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

The electrocaloric (EC) effect describes heating/cooling of a material on adiabatically applying/removing an external electric field. Currently, extensive work in this area is motivated by its huge potential for solid-state cooling devices.

We have performed molecular dynamics simulations for a first principles-based effective Hamiltonian to study the EC effect. In bulk BaTiO_3 , there are three phase transitions – one paraelectric (PE) to ferroelectric (FE) and two FE to FE – with different polarization direction in each FE phase. The EC effect has been mainly studied at the PE to FE phase transition. We calculate the EC temperature change ΔT also at the two FE-FE transitions observed in the bulk. In

particular, we consider the effect of the direction of the applied field on ΔT at each transition. The largest ΔT is observed at the PE-FE transition, however a smaller, but finite effect is also observed at the other two transitions. This is very interesting for applications because one of the FE-FE transitions occurs near room temperature. Further, we observe an “inverse” EC effect, that is, heating on field removal, when the applied field is not along the polarization direction of the ferroelectric phase of the system.

MM 29.4 Wed 11:00 H39

Direct Electrocaloric Effect Measurements in BaTiO_3 -based Ferroelectric Ceramics — ●MEHMET SANLIALP, VLADIMIR V. SHVARTSMAN, and DORU C. LUPASCU — Universität Duisburg-Essen, Institut für Materialwissenschaft

Nowadays small size and high performance of electronic components are highly demanded. However, use of miniaturized high power electronic devices often faces large heat dissipation, which reduces the performance of these devices. Recently, solid-state refrigeration based on the electrocaloric effect (ECE) has been proposed as a promising solution of this problem. ECE is a change of temperature or entropy of a dielectric material under an applied electric field at adiabatic or isothermal conditions, respectively. ECE based refrigerators should combine high efficiency, low cost, be environmental friendly and easy scalable. Therefore, search for materials with large ECE is important. We report on development of two experimental setups to measure the ECE directly: a modified differential scanning calorimeter and a self-made quasi-adiabatic calorimeter. We performed the ECE measurements in several lead-free ferroelectric ceramics: $(1-x)\text{Ba}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3-x(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$, $0.55\text{Ba}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3-0.45(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$ with Fe and Nb doping, $(1-x)\text{Ba}(\text{Sn}_{0.15}\text{Ti}_{0.85})\text{O}_3-x(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$. Temperature, electric field, and composition dependences of the electrocaloric effect have been studied. Furthermore, we compare results of the direct measurements with frequently used indirect estimations based on Maxwell relations to judge the compatibility of these measurement methods.

MM 29.5 Wed 11:15 H39

Electrocaloric Effect in $\text{BaZr}_x\text{Ti}_{1-x}\text{O}_3$: Simulation vs Experiment — ●YANG-BIN MA¹, CHRISTIAN MOLIN², VLADIMIR SHVARTSMAN³, DORU CONSTANTIN LUPASCU³, SYLVIA GEBHARDT², BAI-XIANG XU¹, and KARSTEN ALBE¹ — ¹Technischen Universität Darmstadt — ²Fraunhofer-Institut für Keramische Technologien und Systeme IKTS — ³Universität Duisburg-Essen

The electrocaloric effect (ECE) and the relaxor behavior of $\text{BaZr}_x\text{Ti}_{1-x}\text{O}_3$ (BZT) are investigated as function of Zr content, computationally and experimentally. A lattice-based Ginzburg-Landau-type Hamiltonian is used. A multi-well Landau-type term is applied for unit cells containing Ti, and a single well for Zr. The high-frequency permittivity entering the dipole-dipole interaction is assumed composition-dependent. In experiment, the ECE in BaTiO_3 and BZT ($x = 0.12$ and 0.2) ceramics is studied. The domain patterns are revealed by Piezoresponse Force Microscopy, together with the hysteresis and the ECE at various temperatures. The relaxor behavior is related to the relative standard deviation of the internal field distribution. With increasing Zr content, the domain size becomes smaller, and the hysteresis becomes slimmer. For Zr contents ranging from 0 to 0.3 there is a sharp drop of the ECE peak value, while the drop becomes moderate when Zr contents are larger. Meanwhile, the ECE peak shifts to lower temperature with increasing Zr content, and the temperature change decreases. The phenomena are interpreted explicitly by the domain patterns. It presents a good qualitative consistence between the phenomena observed in simulation and experiment.

15 min. coffee break

MM 30: Structural Materials I

Time: Wednesday 10:15–11:30

Location: H52

MM 30.1 Wed 10:15 H52

Thermodynamic properties of ultra-high temperature ceramics: ab initio accuracy up to the melting point — ●ANDREW DUFF¹, DOMINIQUE KORBMACHER², ALBERT GLENSK², BLAZEJ GRABOWSKI², JOERG NEUGEBAUER², and MICHAEL FINNIS¹ — ¹Department of Materials, Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, UK — ²Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf 40237, Germany

A new method for calculating ab initio thermodynamic properties of materials is presented. The new approach, termed TU-TILD (two-stage upsampled thermodynamic integration using Langevin dynamics) captures the full anharmonicity of the lattice vibrations and provides at least an order of magnitude improvement in efficiency compared to the UP-TILD approach on which it is based. Using TU-TILD, free energies can be calculated up to the melting point at the full accuracy of the underlying ab initio theory— in the present case, density functional theory —overcoming limitations of the widely used quasiharmonic approximation, whilst significantly closing the gap in computational efficiency between fully anharmonic and quasiharmonic methodologies. The new approach is used to calculate thermodynamic properties of the ultra-high temperature ceramics: zirconium carbide; zirconium diboride and hafnium carbide. The results show a distinct improvement over quasiharmonic calculations, with heat capacities and thermal expansion data brought more closely in line with experimental results and, where available, the results of CALPHAD assessments.

MM 30.2 Wed 10:30 H52

Atomic-scale modeling of point defects, phase stability, and the formation mechanism of Z phases CrMN (M=V, Nb, Ta) — ●DANIEL F. URBAN, MATOUS MROVEC, and CHRISTIAN ELSÄSSER — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

The challenge of raising the steam inlet temperature of fossil-fired power plants calls for creep-resistant steels with a Cr content higher than 9% in order to achieve sufficient corrosion and oxidation resistance. However, it has been found that in 11-12% Cr ferritic-martensitic creep resistant steels strengthened by fine (V,Nb)N particles, precipitation of thermodynamically stable Z-phase particles, CrMN (M=V,Nb,Ta), in long-term service is unavoidable and detrimental. Usually, Z-phase particles are coarse and brittle and grow at the expense of the desired fine (V,Nb)N particles.

We present atomistic simulations, using density function theory, which reveal the essential mechanisms underlying the formation of Z-phases. We study the thermodynamic stability of Z-phase, related structures and predecessors as well as the basic phase formation mechanisms. The picture that evolves consists of the diffusion of Cr atoms into MN particles and their subsequent clustering in a layered arrangement which finally yields the transformation of the nitride particles to Z-phase particles. Our results support experimental efforts to control the precipitation of the Z-phase through appropriate microstructural engineering.

MM 30.3 Wed 10:45 H52

Solubility of boron, carbon, and nitrogen in transition metals: getting insight into trends from first-principles calculations — XIAOHUI HU^{1,2}, TORBJÖRN BJÖRKMAN², LITAO SUN¹, and ●ARKADY KRASHENINNIKOV^{2,3} — ¹FEI Nano-Pico Center, Southeast U., China — ²Dep. of Appl.Phys., Aalto U., Finland — ³Helmholtz Zentrum Dresden-Rossendorf, Inst. of Ion Beam Phys. and Mat. Res., Germany

Efficient chemical vapor deposition synthesis of 2D materials such as graphene, boron nitride, and mixed BCN systems requires precise knowledge of the solubility and mobility of B/C/N atoms in the transition metals (TMs) used as substrates for the growth. Yet, surprisingly little is known about these quantities either from experiments or simulations. Using first-principles calculations, we systematically study [1] the behavior of B/C/N impurity atoms in a wide range of TMs. We compute formation energies of B/C/N interstitials and demonstrate that they exhibit a peculiar but common behavior for TMs in different rows of the periodic table, as experimentally observed for C. Our simulations indicate that this behavior originates from an interplay between the unit cell volume and filling of the d- shell electronic states of the metals. We further assess the vibrational and electronic entropic contributions to the solubility, as well as the role of anharmonic effects. Finally, we calculate the migration barriers, an important parameter in the growth kinetics. Our results not only unravel the fundamental behavior of interstitials in TMs but also provide a large body of reference data, which can be used for optimizing the growth of 2D BCN materials. [1] X. Hu, et al., JPC Lett., 6 (2015) 3263.

MM 30.4 Wed 11:00 H52

Modelling yttrium diffusion in ODS steels — ●MARKUS MOCK and KARSTEN ALBE — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

Oxide dispersion strengthened (ODS) steels are promising structure materials for future fission and advanced fusion materials. They contain yttrium oxide nanoparticles that enable outstanding high-temperature properties and unique irradiation tolerance. The size, shape and distribution of the particles is of utmost importance for the properties of the material and understanding the precipitation process will allow tailoring the material properties for specific applications. Precipitation of yttrium oxide particles requires diffusion of yttrium through the iron lattice even though there is a high binding energy between substitutional yttrium atoms and vacancies. To investigate the mechanism of yttrium diffusion we created an atomic bond order potential for the iron-yttrium interaction and calculated activation barriers of relevant diffusion events. We present a model for the diffusion mechanism of yttrium through iron that helps understanding the precipitation process in ODS steels.

15 min. coffee break

MM 31: Functional materials I: Supercapacitors and batteries I

Time: Wednesday 10:15–11:45

Location: H53

MM 31.1 Wed 10:15 H53

Activated Carbon-based Materials of Ultrathin Fibers — ●SVETLANA KLIMOVA — Saratov State University, Astrakhanskaya 83 410012 Saratov, Russia

There is more attention to the development of new autonomous "physical" batteries with energy storage in the electric double layer (ultra-electrolytic capacitors with a dielectric layer between the electrodes (supercapacitors)). Supercapacitor is a new element of energy storage device with energy density 10 times higher than in the conventional capacitors, and pulse discharge capacity up to 10 times higher than the power batteries. High voltage (potential difference), to which the capacitor is charged and capacitance are important in energy area and improve the supercapacitor characteristics. For that present work

new nonwoven materials with/without of inorganic inclusions (carbon or magnetite nanoparticles) are synthesized and modification of porous material to increase the amount of pore is obtained. The electrospinning technology provides continuous production of nanofibrous materials and was used for create a separator of supercapacitors in this work. Morphology and electric parameters were measured by the scanning electron microscope (Tescan Mira LMU II) and probe analyzer (Agilent), respectively. The application of energy storage of condenser type (ESCT) based on supercapacitor energy storage systems with nanofibrous materials makes it possible to reduce the installed capacity batteries and increase their lifetime by 1.5 - 2 times.

MM 31.2 Wed 10:30 H53

Facile synthesis of a δ -bismuth oxide/reduced graphene oxide composite and its electrochemical characteristics — ●BENRONG HAI, YANG XU, MIN ZHOU, and YONG LEI — Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany

The increasing demand for environmentally benign and economically accessible energy storage technologies has strongly promoted the need for scientific work in this area. It is currently accepted that the cubic oxide δ -Bi₂O₃ is one of the most promising materials which can be used as solid electrolyte in high technology equipment such as fuel cells, supercapacitors, and membrane devices which utilize the unusual high oxide ion conductivity of this metal oxide. Reduced graphene oxide is considered as the most excellent matrix to support host materials because of its promising advantages. The present work demonstrates a novel and facile route for preparing composites comprising of δ -Bi₂O₃ nanoparticles and graphene.

MM 31.3 Wed 10:45 H53

NMR parameter computations and the local electronic structure in oxygen-deficient LTO — ●MARKUS SCHUDERER, KARSTEN REUTER, and CHRISTOPH SCHEURER — Theoretische Chemie, Technische Universität München, Garching

Spinel-structured lithium titanium oxide Li₄Ti₅O₁₂ (LTO) is a promising zero-strain anode material for rechargeable lithium ion-batteries. Its relatively low electronic conductivity can be improved by introducing oxygen vacancies [1]. Experimental XPS [1] and EPR [2] results suggest the partial reduction of Ti ions. The description of the respective mixed-valent transition metal cation distribution is challenging for DFT methods. LTO's inherent stoichiometric disorder and the spatial separation of vacancies from periodic images additionally requires large supercells. We have conducted systematic studies employing PBE, DFT+*U*, and hybrid functionals. The expected gap states are only found in hybrid calculations. Computed quadrupolar coupling constants for Li NMR spectroscopy are correlated with local geometric distortions and the electronic structure in the vicinity of O-vacancies, allowing for future combined theoretical and experimental NMR studies of the microscopic ion transfer pathways in this interesting material.

[1] J. Wolfenstine, U. Lee, J. L. Allen, *J. Power Sources* **2006**, *154*, 287.

[2] P. Jakes, J. Granwehr, H. Kungl, R.-A. Eichel, *Z. Phys. Chem.* **2015**, *229*, 1263.

MM 31.4 Wed 11:00 H53

⁷Li NMR studies of lithium ion dynamics in SiOC anode materials — ●MICHAEL HAAKS¹, RALF RIEDEL², and MICHAEL VOGEL¹ — ¹Institut für Festkörperphysik, Technische Universität Darmstadt,

Germany — ²Institut für Materialwissenschaft, Fachgebiet Disperse Feststoffe, Technische Universität Darmstadt, Germany

Rising energy demand makes it important to improve the performance of lithium ion batteries. For this purpose it is important to understand the dynamics of lithium ions, in particular, in heterogeneous materials, which are used in modern strategies for material optimization. We combine ⁷Li NMR spin-lattice relaxation, line-shape, and stimulated-echo analyses to investigate lithium ionic motion in a polymer-derived silicon oxycarbide (SiOC) ceramic in lithiated and delithiated compounds on a broad timescale. We find that the large variety of lithium environments results in broad distributions of correlation times for the jump motion of the lithium ions. Moreover, we observe that the lithium ionic jumps are, on average, faster in the lithiated than in the delithiated compound at ambient temperatures. On the other hand, the lithiated SiOC has a higher temperature dependence of this jumps so that the difference in the ionic mobilities is reduced upon cooling. Finally, we show that heating to 400 K leads to irreversible changes of the prepared lithiated and delithiated samples.

MM 31.5 Wed 11:15 H53

DFT-supported study of ionic mobility in Li₄Ti₅O₁₂ by solid-state NMR — ●SIMONE KÖCHER^{1,2}, MARKUS SCHUDERER², MAGNUS GRAF¹, JOSEF GRANWEHR¹, RÜDIGER-A. EICHEL¹, KARSTEN REUTER², and CHRISTOPH SCHEURER² — ¹IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Jülich, Germany — ²Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool to gain a detailed understanding of the ionic mobility in electrolyte materials. Notwithstanding, the experimental spectra are complex and their unambiguous interpretation has to rely on independent first-principles based calculations. For studies of the ionic charge carrier mobility in Li₄Ti₅O₁₂ (LTO) by ⁷Li spin-alignment echo (SAE) NMR, we provide first-principles reference values for chemical shielding and quadrupolar coupling by density-functional theory (DFT) [1] calculations. The results imply that for a quantification of ion mobility two intrinsically different influences need to be considered. On the one hand, local mobility with fast motion on the experimental timescale partially averages the NMR parameters of interest. On the other hand, global mobility by slower motion between local domains is characterized by effective, residual parameters in NMR. Therefore, the conventional interpretation of ^{6,7}Li chemical shifts and ⁷Li quadrupolar coupling in terms of static lithium occupancy might be incomplete.

[1] C. Bonhomme *et al.*, *Chem. Rev.* **112**, 5733 (2012).

15 min. coffee break

MM 32: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II

Time: Wednesday 10:30–13:00

Location: H24

MM 32.1 Wed 10:30 H24

Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — ●TONGHAO SHEN, ARVID CONRAD IHRIG, IGOR YING ZHANG, and MATTHIAS SCHEFFLER — *Fritz-Haber-Institut der MPG, Berlin.*

For a quantitative prediction of material properties, an advanced description of electronic correlation is crucial. As the "gold standard" correlation method in quantum chemistry, the coupled-cluster (CC) ansatz with singles, doubles and perturbative triples (CCSD(T)) is starting to gain attention in materials science[1]. At present, the CCSD(T)-quality description of the correlation effects in solids can be achieved by either studying the cluster-size convergence toward the bulk in real space[1] or implementing CCSD(T) for extended systems in reciprocal space[2]. In order to investigate and compare these approaches on an equal footing, it is essential to have a computational platform that enables CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. In this report, we present a CCSD(T) implementation for both molecules and solids in the all-electron full-potential code FHI-aims[3] with numeric atom-center orbital (NAO) basis sets. A special memory-distribution strategy is designed to significantly reduce the inter-CPU communication, which is the main challenge for the parallelization of

wave-function methods. The accuracy and efficiency are demonstrated for a group of molecules, 1D-, 2D- and 3D-periodic materials. [1] C. Müller, *et al.*, *PCCP*. **14**, 7605 (2012); [2] A. Grüneis, *et al.*, *JCTC* **7**, 2780 (2011); [3] V. Blum, *et al.*, *CPC* **180**, 2175-2196 (2009).

MM 32.2 Wed 10:45 H24

Surface adsorption energetics at the "gold standard": Small molecule binding to TiO₂(110) — ●DANIEL BERGER^{1,2}, A. KUBAS³, D. MANGANAS³, H. OBERHOFER¹, F. NEESE³, and K. REUTER¹ — ¹TU München — ²University of California, Los Angeles — ³MPI für chemische Energiekonversion, Mülheim an der Ruhr

Adsorption energies at oxide surfaces are central quantities required for catalysis, energy and a multitude of other application areas. At present, the by far dominant computational method to obtain such energetics is density-functional theory (DFT). Unfortunately, systematic benchmarking of such energetics against accurate reference numbers from correlated wave-function theory as known from molecular systems is scarce, largely owing to the fact that the latter techniques are often not available for standard periodic boundary condition supercell calculations.

We address this situation with a solid-state QM/MM embedded cluster approach, in which the adsorbate and immediate surrounding surface atoms are described quantum mechanically, while the long-range

electrostatic interactions are accounted for through a polarizable force field. This yields a numerically highly efficient approach that enables use of the recently developed domain-based local pair natural orbital coupled cluster method with single-, double- and perturbative triple-excitations (DLPNO-CCSD(T)) in the quantum region. We exploit corresponding "gold standard" adsorption energies for a set of prototypical small molecules interacting with the rutile TiO₂(110) surface for a systematic benchmark of DFT numbers.

MM 32.3 Wed 11:00 H24

Water adsorption on surfaces form many-body perturbation theory — ●THEODOROS TSATSIOULIS and ANDREAS GRÜNEIS — Max-Planck-Institute for Solid State Research, Stuttgart

The accurate description of the interaction of molecules with surfaces is of crucial importance for a wide range of phenomena. While Kohn-Sham density functional theory is one of the most widely-used methods for describing the electronic structure of surfaces, many local and semi-local functionals are often not able to produce accurate molecular adsorption energies. Quantum chemical wave-function based methods such as Møller-Plesset perturbation theory (MP2) and coupled-cluster methods promise controllable accuracy, however, at much higher computational costs. Large part of the latter is due to the number of virtual states. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves, leading to reduced computational cost. In particular we study water adsorption on bulk LiH and h-BN sheets at the level of MP2 theory within the projector-augmented-wave method as implemented in VASP [1]. The results are compared to state-of-the-art methods such as hybrid functionals and diffusion Monte Carlo [2].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)

[2] Al-Hamdani et al., The Journal of Chemical Physics, 142, 181101 (2015)

MM 32.4 Wed 11:15 H24

Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — ●CATERINA COCCHI and CLAUDIA DRAXL — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols on gold suffer from hindered photo-isomerization, as observed experimentally [1]. While this behavior is generally ascribed to strong intermolecular coupling, a clear microscopic understanding of this phenomenon is still missing. In order to address this question, we perform a first-principles study of the excited-state properties of azobenzene-functionalized SAMs. In the framework of many-body perturbation theory (GW approximation and Bethe-Salpeter equation), as implemented in the all-electron full-potential code exciting [2], we investigate the optical absorption spectra of these materials, inspecting the influence of packing density and functionalization of the azobenzene molecules with different end groups. Through a systematic analysis of the character of the excitations, we clarify the role and interplay of screening and local-field effects, which strongly impact light absorption and hence photo-isomerization in these systems.

[1] C. Gahl et al. J. Am. Chem. Soc. 132, 1838 (2010). [2] A. Gulans et al. J. Phys.: Condens. Matter 26, 363202 (2014).

MM 32.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — ●ARVID CONRAD IHRIG¹, PATRICK RINKE², IGOR YING ZHANG¹, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²Aalto University, Helsinki, Finland

A well-known problem in local and semi-local density functional approximations and to a lesser extend also in hybrid functionals is the one-electron self-interaction error, which can lead to a qualitatively wrong description for applications like charge-transfer systems. One possible remedy is the 2nd order Møller-Plesset perturbation theory (MP2), which does not suffer from this error. However, the time and memory requirements for MP2 prevent its routine-use for large molecular and periodic systems. The Laplace-transformed MP2 (LT-MP2) [1] can significantly reduce the computational time, but requires the usage of intermediate variables stored on disk, resulting in an inefficient usage of computational resources. In this work we combine the LT-MP2 with our localized Resolution of Identity (RI-LVL) [2] approach to eliminate the disk-storage bottleneck and fully exploit massive par-

allelization strategies. RI-LVL expands the basis function pairs in the electron repulsion integrals in local auxiliary basis sets. For the example of water clusters, we demonstrate the favourable memory scaling (at worst N^2) of our new MP2 implementation, which facilitates the in-memory calculation of large systems at high accuracies.

[1] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)

[2] Ihrig et al., New J. Phys. 17, 093020 (2015)

MM 32.6 Wed 11:45 H24

GW singles contributions for the random phase approximation correlation energies — ●JIRI KLIMES¹, MERZUK KALTAK², EMANUELE MAGGIO³, and GEORG KRESSE³ — ¹J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — ²Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — ³University of Vienna, Faculty of Physics, Vienna, Austria

The random phase approximation (RPA) to the correlation energy yields often very accurate results for condensed matter systems. However, a general tendency to underbind has been observed for systems such as molecular solids or for adsorption. One of the ways that have been proposed to improve the accuracy of RPA are the so-called singles corrections of Ren and coworkers [1]. We present our derivation of the singles corrections using the assumption that the electron density changes when going from the reference to the interacting system [2]. This leads to a very compact expression for the corrections. Moreover, the singles formula can be easily modified to account for screening effects, giving the *GW* singles. We assess the effect of both the original and modified singles on covalently and metallically bonded systems as well as on simple weakly bonded systems. Finally, we show that adding the singles corrections leads to considerably improved adsorption energies and lattice energies of molecular solids.

[1] Ren, Tkatchenko, Rinke, Scheffler, Phys. Rev. Lett **106**, 153003 (2010).

[2] Klimes, Kaltak, Maggio, Kresse, J. Chem. Phys. **143**, 102816 (2015).

MM 32.7 Wed 12:00 H24

Long-range corrected DFT meets GW: Vibrationally resolved photoelectron spectra from first principles — ●THOMAS KÖRZDÖRFER — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

We introduce an entirely non-empirical and computationally efficient scheme to calculate highly reliable vibrationally resolved photoelectron spectra for molecules from first principles.[1] To this end, we combine non-empirically tuned long-range corrected hybrid functionals with non-self-consistent many-body perturbation theory in the G_0W_0 approximation and a Franck-Condon multi-mode analysis based on DFT-calculated frequencies. The vibrational analysis allows for a direct comparison of the GW-calculated spectra to gas-phase ultraviolet photoelectron measurements of neutral and anionic molecules, respectively. In addition, vertical IPs and EAs were benchmarked against other *GW* methods and basis-set extrapolated CCSD(T) results for a recently introduced test set of 24 molecules frequently used in organic electronics.[2] $G_0W_0@LRC$ -DFT yields mean absolute errors on the order of 0.1 eV for IPs, EAs, and fundamental gaps, clearly outperforming commonly used G_0W_0 approaches as well as partially and fully self-consistent *GW* methods.

[1] L. Gallandi and T. Körzdörfer, JCTC **11**, 5391 (2015).

[2] L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer, JCTC *accepted for publication* (2015).

MM 32.8 Wed 12:15 H24

LDA-1/2 as a starting point for G_0W_0 calculations — ●RONALDO RODRIGUES PELA^{1,2}, UTE WERNER¹, DMITRII NABOK¹, and CLAUDIA DRAXL¹ — ¹Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Berlin, Germany — ²Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

For many semiconductors and insulators, LDA represents a bad starting point for G_0W_0 calculations. Hybrid functionals improve upon LDA, but at the price of increasing computational cost of about 2 orders of magnitude. An alternative starting-point for the single-shot G_0W_0 can be the LDA-1/2 method [1], because it approximately includes the self-energy of quasi-particles within a generalized Kohn-Sham scheme, leading to improved band-gaps over the LDA ones, but without being computationally more involved. In this work, we systematically compare 3 starting-points for G_0W_0 calculations: LDA, PBE0, and the LDA-1/2 method. A selection of semiconductors (C, Si, SiC, AlP, LiF, MgO, Ne, Ar, GaN, GaAs, CdS, ZnS, and ZnO) is

chosen for this benchmark. We demonstrate that LDA-1/2 is a good choice in most cases, reducing the root mean square error in band-gap predictions by 50% when compared to G_0W_0 on top of LDA or PBE0. With the exception of large band gap materials, LDA-1/2 predictions are already close to the experimental band gaps, and thus G_0W_0 has minor effects.

Reference [1]: Phys. Rev. B 78, 125116 (2008).

Acknowledgements: “Coordenação de Aperfeiçoamento de Pessoal de Nível Superior” (CAPES) and “Alexander von Humboldt Stiftung”.

MM 32.9 Wed 12:30 H24

DFT+U within a numeric atom-centered orbital basis — ●MATTHIAS KICK, HARALD OBERHOFER, and KARSTEN REUTER — Technische Universität München

Materials like transition metal oxides (TMOs) still challenge a description through first-principles density-functional theory (DFT). Appropriately capturing the electron localization in TMOs generally requires at least hybrid exchange-correlation functionals. Such higher-rung functionals come with appreciable computational cost, which limits their use in large supercell calculations. For such applications effective and numerically less intense approaches are therefore still a much sought alternative.

One such method is the DFT+U approach, where the on-site Coulomb correlation effects are treated using a model Hamiltonian, while remaining interactions are treated on the level of semi-local DFT. Full DFT+U functionality including nuclear gradients (forces) has been implemented in the electronic structure code *FHI-aims*. We account for three common occupation matrix representations, differing in the way how the occupations of the correlated subspaces are determined. We critically discuss their performance and differences in the context of the numeric atomic orbital basis sets employed in *FHI-aims*.

The established numerically efficient framework is finally used to address neutral and charged oxygen vacancies at the $\text{TiO}_2(110)$ surface within a solid-state embedding approach.

MM 32.10 Wed 12:45 H24

High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides — ●CHRISTOPHER SUTTON, LUCA M. GHIRINGHELLI, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Ternary Al, Ga, and In-based sesquioxides are investigated as alternative wide-bandgap semiconductors motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in $(\text{GayIn}_{1-y})_2\text{O}_3$ from 3.8 eV to ca. 5 eV [1] and ca. 5 eV to 7.5 eV for $(\text{Al}_{1-x}\text{Ga}_x)_2\text{O}_3$ [2].

New ternary oxides with the chemical structure of $(\text{Al}_x\text{GayIn}_{1-x-y})_2\text{O}_3$ have been identified using cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search potential (ordered and disordered) configurations within a given lattice and for different temperatures. Wang-Landau and diffusive nested sampling has also allowed for a consideration of the effect of entropy on the relative stability of ternary oxides. Statistical learning has also been used to identify a structure-property relationship to efficiently identify new wide-band gap TCOs to improve the fundamental chemical and physical properties (e.g., conductivities, mobilities, and optical transparency) by investigating the parameters that control these properties.

[1] F Zhang, et al., Solid State Communications 2014, 186, 28. [2] H Ito, et al., Japanese Journal of Applied Physics 2012, 51, 100207.

MM 33: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science III - Atomic structure and defects II

Time: Wednesday 11:45–13:15

Location: H38

Topical Talk

MM 33.1 Wed 11:45 H38

Deformation mechanisms of grain boundaries in Al and TiAl from atomistic simulations — ●REBECCA JANISCH — ICAMS, Ruhr-Universität Bochum, Germany

Interfaces in metallic micro- and nano-structures play a role during plastic deformation in many respects. Besides accommodating part of the plastic strain by means of grain boundary sliding and migration they can act as sources, sinks, or barriers for dislocations, as well as crack nucleation sites. These processes are not independent, and often several of them occur at the same time. To isolate the intrinsic deformation mechanisms of grain boundaries we have carried out molecular statics and molecular dynamics simulations of bi-crystal shear at different interfaces in Al and TiAl. Four distinct mechanisms could be identified, namely rigid grain sliding, grain boundary migration, coupled sliding and migration, and dislocation nucleation and emission. Depending on the loading direction different mechanisms can occur at one and the same grain boundary, i.e. there is a pronounced anisotropy in the interfacial shear behaviour. This anisotropy is suggested as the explanation for seemingly contradicting experimental results on the role of grain boundary sliding during creep of lamellar TiAl alloys. By varying the geometry and chemistry of the interfaces we could relate the observed mechanisms to structural features of the grain boundaries as well as to physical properties of the material. The influence of external factors such as strain and temperature will be discussed in the presentation.

MM 33.2 Wed 12:15 H38

X-ray microdiffraction Laue experiments to understand plasticity at interfaces — ●CHRISTOPH KIRCHLECHNER^{1,2}, NATALIYA MALYAR¹, PETER IMRICH², and GERHARD DEHM¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²University of Leoben, Leoben, Austria

The deformation behavior of metallic single crystals is size dependent, as shown by several studies during the last decade (Uchic et al. 2009, Greer and De Hosson 2011). Nevertheless, real structures exhibit different interfaces like grain, twin or phase boundaries. Due to the possibly higher stresses at the micron scale, the poor availability of dislo-

cation sources and the importance of diffusion in small dimensions the mechanical behavior of samples containing interfaces can considerably differ from bulk material. In the talk we show the first in situ microdiffraction Laue compression experiments on micron sized, bi-crystalline samples. Three different grain-boundary types will be presented and discussed (i) Large Angle grain Boundaries (LAGBs) acting as strong obstacle for dislocation slip transfer; (ii) LAGBs allowing for easy slip transfer and (iii) coherent σ_3 twin-boundaries. The talk will focus on pile-up of dislocations at the boundary, slip transfer mechanisms, storage of dislocations and dislocation networks at the LAGB.

MM 33.3 Wed 12:45 H38

Quantitative measurements of grain boundary excess volume from HAADF-STEM micrographs — YULIA BURANOVA, ●HARALD RÖSNER, SERGIY DIVINSKI, and GERHARD WILDE — WWU Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

A novel approach for quantitative measurements of grain boundary excess volume has been developed combining several electron scattering signals and successfully demonstrated for several simulated symmetrical [100] tilt GB configurations as well as for the experimental case of an Al bicrystal containing a near $\Sigma 13$ GB with an additional twist component. The reliability and precision of this new approach is analyzed and the limitations are discussed.

The authors are grateful to Prof. D. Molodov (Institut für Metallkunde und Metallphysik, RWTH Aachen, Germany) for providing Al bicrystals and acknowledge partial funding through a DFG grant (SPP 1713).

MM 33.4 Wed 13:00 H38

In-situ investigations with high-energy X-ray diffraction of the diffusion brazing process of γ -TiAl alloys — ●KATJA HAUSCHILD, ANDREAS STARK, NORBERT SCHELL, URSULA TITZ, HELMUT ECKERLEBE, FLORIAN PYCZAK, and MARTIN MÜLLER — Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, 21502 Geesthacht

Diffusion brazing is a promising method to close cracks (in noncrit-

ical or not highly loaded areas) in parts made of TiAl alloy, as for example aero engine vanes. In this work the phase constituents, phase distribution, and microstructure of the joint zone of diffusion brazed Ti-45Al-5Nb-0.2B-0.2C (in at. %) alloys are investigated. Two brazing alloys based on Ti-Fe and Ti-Ni are used.

The phases and their distribution in the brazing zone were determined time and space resolved by high-energy X-ray diffraction (HEXRD) using the materials science beamline HEMS at the PETRA

III synchrotron radiation facility at DESY in Hamburg, Germany.

Therefore, the brazing zone was scanned in several steps over the joint while heating.

The results show, that different phases occur over time in the Ti-Ni joint. In contrast the phase constitution in the Ti-Fe joint shows only little change over time. In comparison, scanning electron microscopy was used to characterize the microstructures of the two systems after brazing.

MM 34: Topical session: Caloric effects in ferroic materials IV - Heuslers

Time: Wednesday 11:45–12:45

Location: H39

MM 34.1 Wed 11:45 H39

Nucleation barrier of martensite in magnetocaloric Heusler films — ●ROBERT NIEMANN^{1,2}, ANETT DIESTEL¹, ANJA BACKEN¹, SANDRA HAHN³, MARTIN F.-X. WAGNER³, LUDWIG SCHULTZ^{1,2}, and SEBASTIAN FÄHLER^{1,2} — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — ²Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, D-01062 Dresden, Germany — ³Technische Universität Chemnitz, Institute of Materials Science and Engineering, D-09107 Chemnitz, Germany

Martensitic transformations in magnetic shape memory alloys lead to large temperature- and field-dependence of the magnetization and accordingly to large entropy changes. These ferroic materials are discussed for applications in solid-state cooling cycles, but only if the thermal hysteresis can be reduced. Therefore it is important to understand the origin of hysteresis and to differentiate the contributions of nucleation and growth. As a model system we study epitaxial thin films of Heusler alloy Ni-Mn-Ga-(Co). The shape of the nucleus is known from in-situ experiments. We calculate the theoretical barrier for homogeneous nucleation using a continuum model of the nucleus and employing classical nucleation theory. From time-dependence of the magnetization we can identify growth and nucleation events and calculate the respective energy barriers. The energy necessary for nucleation is also derived from the difference between full and minor loops of the transformation. We conclude that only heterogeneous nucleation is possible and show that the barrier is effectively reduced by nanoindentation. Funded by DFG SPP1599 www.FerroicCooling.de

MM 34.2 Wed 12:15 H39

Impact of point defects on the phase stability in Heusler alloys: A first-principles study — ●BISWANATH DUTTA, VIJAYA BEGUM, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Functional properties of magnetic Heusler alloys such as magnetic shape memory and magnetocaloric effect depend critically on their thermoelastic martensitic transformation. To this end, vacancies can play a decisive role as they control the ordering kinetics in these materials, which has recently been confirmed in experiments. Within this

study, we employ density functional theory along with Monte Carlo (MC) simulations to understand the impact of vacancies on the phase stability and transformation behavior in Ni-Mn-based Heusler alloys. Our calculations reveal high vacancy concentrations for Ni and Mn with the vacancy formation energy for Ni being the lowest. We discuss the results in terms of chemical potentials obtained against the formation of different unary and binary phases. The nudged elastic band method is employed to compute the vacancy migration barrier. Our calculated results for the self-diffusion activation energy of vacancies show good agreement with experimental values. Using these results as input for MC simulations we discuss the impact of vacancies on the ordering tendency in these materials.

MM 34.3 Wed 12:30 H39

Magnetocaloric and microstructural properties of Half-Heusler-type alloys — ●ANDREAS TAUBEL, TINO GOTTSCHALL, KONSTANTIN P. SKOKOV, ILIYA A. RADULOV, and OLIVER GUT-FLEISCH — Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Magnetocaloric refrigeration offers an efficient and environmentally friendly alternative to conventional gas compression cooling. Besides the well-known Gd-Si-Ge and La-Fe-Si systems, Heusler alloys and their related Half-Heusler and MM'X materials come into focus. The Mn-Ni-Ge system exhibits a martensitic phase transition from its high temperature hexagonal phase to its low temperature orthorhombic phase with a broadly tunable transition temperature when partially substituting Fe for Mn or Ni. Previous studies already showed a sharp transition with low hysteresis and considerable changes in magnetization during the transition. In this work, we could obtain very large isothermal entropy changes ΔS_m of up to $-37.8 \text{ Jkg}^{-1}\text{K}^{-1}$ based on magnetic measurements of small single pieces. However the high volume change of 2.7 % results in an embrittlement of large particles into several smaller grains. For this reason bonding of the material with a polymer epoxy was carried out in order to enable direct measurements of ΔT_{ad} and to evaluate the possibility for its usage under real conditions in a magnetocaloric cooling device.

Supported by DFG Priority programme 1599

MM 35: Structural Materials II

Time: Wednesday 11:45–12:45

Location: H52

MM 35.1 Wed 11:45 H52

First-principles study of carbon segregation in bcc iron symmetrical tilt grain boundaries — ●JINGLIANG WANG, GEORG K. H. MADSEN, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, D-44801, Bochum, Germany

Using density functional theory (DFT), we studied the C segregation behavior to three low- Σ symmetrical tilt grain boundaries (STGBs) in bcc-Fe. For each GB, we examined potential segregation sites and demonstrated that the most stable segregation sites always possess the greatest coordination number and maximum nearest Fe-C neighbor distance. Thereby a geometric criterion for predicting the segregation sites for more general GBs is suggested. We rationalized the geometric criterion by splitting the solution energy into chemical and mechanical contribution. The chemical contribution is shown to be related to the coordination number, whereas the mechanical contribution is related to the Fe-C bond length. The effect of C on the GB energies depends on the GB structure. The open GBs are stabilized by C seg-

regation and the GB energy continuously decreases by increasing the C concentration while the compact GB shows an opposite trend.

MM 35.2 Wed 12:00 H52

Origin of the off-stoichiometry of Fe-Mn-Al-C kappa carbides: An ab-initio explanation of atom probe tomography data — ●POULUMI DEY¹, ROMAN NAZAROV², BISWANATH DUTTA¹, MENGJI YAO¹, MICHAEL HERBIG¹, MARTIN FRIÁK³, TILMANN HICKEL¹, DIERK RAABE¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — ²Livermore National Laboratory, Livermore, CA 94550, USA — ³Institute of Physics of Materials, v.v.i., Academy of Sciences of the Czech Republic, CZ-61662 Brno, Czech Republic

Quaternary Fe-Mn-Al-C alloys have exceptional mechanical properties such as high strength and ductility. In a certain composition range these alloys show a microstructure that comprises of an austenitic Fe-based matrix along with regularly arranged nano-sized kappa carbides

which strongly strengthens the material. The nominal composition of kappa carbide is $(\text{Fe},\text{Mn})_3\text{AlC}$, but our atom probe tomography measurements have indicated reduced C and Al contents in these carbides. Using density functional theory calculations, we succeeded to explain the experimentally observed off-stoichiometry with respect to C as a consequence of minimizing the elastic strains emerging in coherent microstructures. The off-stoichiometric concentration of Al can also be explained to a certain extent by a strain minimization caused by Mn antisite defects on the Al sub-lattice in kappa carbide. However, this effect becomes only significant if C vacancies are present in the vicinity of the antisite. We therefore demonstrated that the phenomena of depleted interstitial C and substitutional Al are coupled.

MM 35.3 Wed 12:15 H52

Structure of the high entropy alloy $\text{Al}_x\text{CrFeCoNi}$: fcc versus bcc — •MASAKO OGURA¹, TETSUYA FUKUSHIMA², RUDOLF ZELLER¹, and PETER H. DEDERICHS¹ — ¹Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — ²Graduate School of Engineering Science, Osaka University, Toyonaka, Japan

High entropy alloys (HEAs) are disordered multi-component systems with equal or near-equal atomic ratios. They have simple solid solution structures, e.g., bcc and fcc structures, stabilized by the high disorder entropy effect. The structure of HEAs with Al such as $\text{Al}_x\text{CrFeCoNi}$ and $\text{Al}_x\text{CrFeCoNiCu}$ changes from fcc to bcc with increasing the Al concentration. In this study, we investigate the effect of Al on the structure of the HEA $\text{Al}_x\text{CrFeCoNi}$ on the basis of first-principles electronic structure calculations. The calculations are performed with the

KKR Green's function method in the framework of the density functional theory using GGA. The disordered alloys are simulated by the coherent potential approximation or supercell calculations with several hundred atoms. We discuss the change from fcc to bcc structures and the importance and stability of partially disordered B2 and L1₂ structures.

MM 35.4 Wed 12:30 H52

First-principles investigations on intermetallic $\epsilon\text{-Al}_5\text{Fe}_2$ phase — •LILIT AMIRKHANYAN and JENS KORTUS — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

The iron-aluminum system is of commercial and technical interest, as it has low density, high thermal conductivity, high strength and formability. The $\epsilon\text{-Al}_5\text{Fe}_2$ structure is a high-temperature phase in the Al-Fe binary system, which is stable between 1368 K - 1504 K [1].

We investigated the $\epsilon\text{-Al}_5\text{Fe}_2$ intermetallic phase, using density functional theory (PAW pseudopotential) calculations in order to understand the Al and Fe preferred sites. Our study focused on four different possible crystallographic site changes between Al-Fe positions. For each case we optimized the structure, minimizing the ground-state energy, the atomic forces and the stresses. This structure was then used to calculate the bulk module. The elastic properties contain information on the stability of the investigated structures. Further, we investigated the magnetism in the phase.

References

1. Vogel, SvenC. and Stein, Frank, P.Martin. Applied Physics A **99**(3), [607-611], 2010

MM 36: Functional materials II: Batteries II

Time: Wednesday 11:45–13:00

Location: H53

MM 36.1 Wed 11:45 H53

Phase field modeling of Li-insertion kinetics in single LiFePO_4 – nano-particles for rechargeable Li-ion battery application — •MICHAEL FLECK, PHILIPP AMENDT, HOLGER FEDERMANN, and HEIKE EMMERICH — Materials and Process Simulation, University of Bayreuth, Germany

LiFePO_4 is widely considered to be a promising cathode material for Li-ion rechargeable batteries. The lithiation process in LiFePO_4 – nano-particles proceeds via a coherent solid-solid phase transformation between the LiFePO_4 (LFP-phase) and FePO_4 (FP-phase). We develop a continuum phase field model for solid-solid phase transformations in single- LiFePO_4 – nano-particles, embedded in an elastically soft electrolyte-phase. The model-description explicitly includes anisotropic (orthorhombic) and inhomogeneous elastic effects, resulting from coherency strain, as well as anisotropic (1D) Li-diffusion insight the nano-particles. The moving LFP/FP-phase boundary is modeled as a diffuse interface of finite width. Here, with the inclusion of the elastically soft electrolyte-phase, we consider also non-rectangular shaped LiFePO_4 – particles in a fully anisotropic 3D-framework. The resulting model is employed to investigate effects of the nano-particle's size and shape on the kinetics of FP to LFP phase transformations, relating to single particle charge rates. In respective model studies, we find that in flat particles the transformation velocity increases over more than two orders of magnitudes with decreasing particle-height. We show that in contrast to Cahn-Hilliard-type models this behavior can be regularized in Allen-Cahn-type phase-field formulations.

MM 36.2 Wed 12:00 H53

Charge localization and energetics of Li-ion batteries cathodes from Hubbard-corrected DFT functionals — MATTEO COCCIONI and •NICOLA MARZARI — EPFL, Lausanne, Switzerland

An accurate modeling of the electronic, magnetic and structural properties of transition-metal (TM) compounds is essential for their deployment in many emerging technologies. Unfortunately, the importance of electronic correlations makes first-principles calculations on these systems very challenging. This is particularly true for Li-ion battery materials and for all the electrochemical energy conversion and storage applications based on mixed-valence TM ions. DFT functionals augmented with corrective terms based on the Hubbard model (DFT+U) improve significantly the description of these correlated materials and have proven themselves as the standard choice when high

computational efficiency is required (e.g., for screening large numbers of compounds). This work shows how an extended formulation of DFT+U, including on-site (U) and inter-site (V) interactions, improves the description of mixed-valence materials. Focusing on Li_xFePO_4 and Li_xMnPO_4 we discuss their structural and electronic properties in dependence of Li content. Contradicting common practice, we also show that using computed interaction parameters is actually crucial to reliably compare the energy of different Li concentrations and, in particular, to assess the thermodynamic stability of various compositions and to evaluate the voltage of the resulting battery.

MM 36.3 Wed 12:15 H53

Ab-initio based continuum parameters for phase separating Li battery materials — •NICOLAS G. HÖRMANN^{1,2} and AXEL GROSS^{1,3} — ¹Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, Helmholtzstr. 11, 89069 Ulm — ²THEOS, EPFL, Switzerland — ³Universität Ulm, Institut für Theoretische Chemie, Albert-Einstein-Allee 11, 89069 Ulm

Modelling of battery materials is getting increasing attention due to the importance of understanding and improving electrochemical energy storage systems. Electrode properties have been studied widely both by ab-initio computations and within continuum models based on experimental parameters [1-3]. It would be desirable, however, to obtain continuum parameters based on ab-initio computations, firstly, to compare results on both scales and understand better the limitations of each approach, and secondly, to estimate the behavior of materials not yet known from experiment.

In this talk, we present a scheme to derive continuum parameters, in particular the mean field homogeneous free energy, from ab-initio calculations based on density functional theory (DFT) for the two phase separating materials LiFePO_4 and $\text{Li}_2\text{FeSiO}_4$. We will also test the quantitative accuracy against experimental results for properties such as the phase diagram and the expected voltage hysteresis.

[1] R. Malik et al., *J. Electrochem. Soc.*, **160**, 5, A3179-A3197 (2013)
[2] R. Malik et al., *Nat. Mater.*, **10**, 587-590 (2011) [3] D. A. Cogswell et al., *Nano Lett.*, **13**, 3036-3041 (2013)

MM 36.4 Wed 12:30 H53

Highly Conductive Interfaces: A Key Factor for Solid State Lithium Batteries — •YASER HAMED JΟΥYBARI and FRANK BERKEMEIER — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Germany

Thin film lithium ion batteries have been in focus during the last years, e.g. due to their prospective capability of carrying high energy densities. However, their development is facing some major challenges such as the synthesis of highly conductive solid state electrolytes and highly conductive interfaces between the electrolyte and the electrodes.

Hence, in this work lithium phosphorous oxynitride (LiPON) layers are prepared via rf magnetron sputtering, serving as a potential solid state electrolyte in future thin film batteries. First, the influence of different sputter parameters on the properties of the LiPON is investigated, to obtain optimized LiPON layers of highest achievable conductivity. Afterwards, the interface adhesion and conductivity between LiPON and different electrode materials is studied. Within these studies it is found that the lithium transport through the interface between LiPON and the electrode material strongly depends on the interface adhesion and the interface bonding conditions. These can be controlled by the sputter parameters during LiPON deposition. Therefore, the dependence of the morphological and electrochemical properties of the layer stacks on the processing parameters is characterized in detailed and explained, theoretically. Finally, by applying optimum processing parameters, LiPON coated electrodes are prepared which exhibit

a high interface conductivity and excellent storage capacities.

MM 36.5 Wed 12:45 H53

Local Structure, Transport and Phase Transformation in Lithium Manganese Dioxide — ●CARSTEN NOWAK, JONAS ARLT, TORBEN ERICHSEN, JOHANNES MAIER, BJÖRN PREIFFER, and CYNTHIA A. VOLKERT — Georg-August-Universität Göttingen, Institute for Materials Physics, Göttingen, Germany

Local structure, ionic and electronic transport, and phase transformations are crucial for the interconversion of electrical and chemical energy in Lithium Manganese Oxide (LMO). Although the material is widely used for electrochemical energy storage, transport and conversion mechanisms at the atomic scale are not fully understood.

Here, we present experimental results on the local characterization of structure, transport and phase transformations in LMO using transmission electron microscopy (TEM) and atom probe tomography (APT). Combining different analytical techniques and in-situ experiments, the Lithium content of LMO is changed and the response of the material is characterized on nanometer length scales. Results are discussed in view of electrochemical energy storage.

MM 37: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III

Time: Wednesday 15:00–18:30

Location: H24

Topical Talk MM 37.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — TOMÁŠ RAUCH¹, STEVEN ACHILLES¹, ●JÜRGEN HENK¹, and INGRID MERTIG^{1,2} — ¹Martin Luther University Halle-Wittenberg, Halle, Germany — ²Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of “original” TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ± 1 ; their projections onto the surface Brillouin zone are connected by a Fermi arc, i.e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained HgTe_{1-x}S_x alloys [1], with surprising results. (i) In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x . (ii) On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the “topological playground” for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk MM 37.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — ●BINGHAI YAN — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monpnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B **92**, 115428 (2015). [2] L. X. Yang, et al. Nature Physics **11**, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics **11**, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

MM 37.3 Wed 16:00 H24

Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe₂ — ●LUKAS MUECHLER¹, ARIS ALEXANDRADINATA², TITUS NEUPERT³, and ROBERTO CAR¹ — ¹Dept. of Chemistry, Princeton University — ²Dept. of Physics, Yale University — ³Princeton Center for Theoretical Science, Princeton University

WTe₂ is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm²/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe₂ based on Wannier functions from *ab-initio* calculations and extend our findings to the iso-structural compounds MoTe₂ and ZrI₂.

MM 37.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — ●YAN SUN¹, SHU-CHUN WU¹, CLAUDIA FELSER¹, and BINGHAI YAN^{1,2} — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully *ab initio* calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

- [1] L. X. Yang, Z. K. Liu, Y. Sun, et. al. Nat.Phys.11,728, (2015).
- [2] Z. K. Liu, L. X. Yang, Y. Sun, et.al Nat. Mater., doi:10.1038/nmat4457,(2015).
- [3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, **92**, 115428, (2015).

MM 37.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — ●L NICOLAI^{1,2,3}, K HRICOVINI^{2,3}, J-M MARIOT⁴, M C RICHTER^{2,3}, O HECKMANN^{2,3}, U DJUKIC², T BALASUBRAMANIAN⁵, M LEANDERSSON⁵, J SADOWSKI⁵, J DENLINGER⁶, I VOBORNIK⁷, J BRAUN⁷, H EBERT⁷, and J MINAR^{7,8} — ¹LMU, Munich — ²LPMS, UCP, Cergy, France — ³DSM-IRAMIS, Spec, Cea-Saclay, France — ⁴LCP-MR, UPMC Univ. Paris 06/CNRS, France — ⁵MAX-lab, Lund Univ., Sweden — ⁶ALS, Berkeley, USA — ⁷EST, Trieste, Italy — ⁸Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states.[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

MM 37.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from GW calculations — ●TOBIAS FÖRSTER, PETER KRÜGER, and MICHAEL ROHLFING — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi₂Se₃, Bi₂Te₃, and Sb₂Te₃ with thicknesses from one to six quintuple layers employing the GW method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing \mathcal{H}^{QP} . The origin of the respective off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in GW differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

MM 37.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — ●STEFAN KURTH^{1,2} and GIANLUCA STEFANUCCI^{3,4} — ¹Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — ²IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — ³Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — ⁴INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

MM 37.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations —

●GIUSEPPE FOTI and HECTOR VAZQUEZ — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)

[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

MM 37.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — ●ZHI WANG¹, SHU-SHEN LI², and LIN-WANG WANG³ — ¹Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — ²Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — ³Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~ 0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge separations in photovoltaic systems.

MM 37.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — ●RYAN REQUIST and EBERHARD K. U. GROSS — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions “smear out” the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys. Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

MM 37.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — ●JAN MINAR^{1,2}, JURGEN BRAUN¹, and HUBERT EBERT¹ — ¹LMU München, Germany — ²University of West Bohemia, Plzeň, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi₂Se₃ band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

MM 37.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — ●THORSTEN DEILMANN, MATTHIAS DRÜPPEL, and MICHAEL ROHLFING — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.

We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used GW method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.

We investigate trion states in a semiconducting (8, 0) carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by ~ 135 meV compared to the excitons.

MM 38: Invited talk Pastewka

Time: Wednesday 15:00–15:30

Location: H38

Invited Talk MM 38.1 Wed 15:00 H38
Models for adhesion, friction and wear across the scales — ●LARS PASTEWKA¹, PETER GUMBSCH^{1,2}, MICHAEL MOSELER², GIANPIETRO MORAS², ANKE PEGUIRON², and MARK ROBBINS³ — ¹Karlsruhe Institute of Technology, Institute for Applied Materials, Karlsruhe, Germany — ²Fraunhofer IWM, Freiburg, Germany — ³Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, USA

Adhesion, friction and wear are processes where the surface of a material plays a central role. Studying these processes is made complicated by most surfaces rough topography, their interaction with the environment, and the inaccessibility of the interface between two materials to *in situ* experimental techniques. In this talk, I give exam-

ples of how computer simulations at mesoscopic to atomic scales can help to elucidate the processes that take place at these buried interfaces. Mesoscopic simulations of elastic contact between randomly rough surfaces allow a direct calculation of the area of intimate atomic contact and reveal emergence of macroscopic adhesion as a function of topography and microscopic surface forces. Conditions within the contacting regions are typically extreme and give rise to severe plastic deformation and change of the material microstructure. Atomic-scale calculations based on classical molecular dynamics, tight-binding and density-functional theory under such conditions reveal how this “tribomutation” evolves in diamond and amorphous carbon, and how its formation facilitates wear of these materials in contact with each other and in contact with oxide ceramics.

MM 39: Biomaterials and Biopolymers I (joint session CPP/BP/MM)

Time: Wednesday 15:00–18:15

Location: H40

MM 39.1 Wed 15:00 H40
Self-assembled plasma protein nanofibers — ●CHRISTIAN HELBING¹, TANJA DECKERT-GAUDIG², and KLAUS D. JANDT¹ — ¹Chair of Materials Science, Department of Materials Science and Technology, Otto Schott Institute of Materials Research (OSIM), Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Jena, Germany — ²Institute for Photonic Technology, Jena, Germany

Protein nanofibers (PNFs) are promising materials for numerous applications in the field of biomedical engineering. Especially, self-assembled PNFs based on plasma proteins have a high importance due their easy fabrication and high biocompatibility. However, knowledge about the self-assembly mechanism of such PNFs is limited. The aim of the current study is to deepen the understanding of the formation mechanism. We tested the hypotheses that morphology and inner structure of PNF depends on environmental conditions. In this work, we present results of self-assembled PNF structures formed in solution from a plasma protein combination. The observed morphology of the formed PNFs depended strongly on the formation conditions. The structural analysis suggest that a partial denaturation, i.e. a change in the secondary structure, of the plasma proteins is a necessary requirement for the formation of PNFs. The comparison of the secondary structure of the PNFs and the native proteins helps to improve the understanding of the self-assembly mechanism. The current results leads to a better control during the PNF formation.

MM 39.2 Wed 15:15 H40
Automatically recognizing structural patterns in (bio)polymers — ●MICHELE CERIOTTI — École Polytechnique Fédérale de Lausanne

Atomistic simulations have been constantly increasing in accuracy and predictive power over the past decade, and materials and molecules of growing complexity are now amenable to modelling. There is however a dire need for algorithms to analyze the outcome of such simulations, to infer the elementary building blocks and the design principles that link atomic-scale structure and the emergence of meso-scale complex behavior. Here I will show how a probabilistic analysis of molecular motifs (PAMM) algorithm can be used to automatically recognize secondary structure patterns in proteins, and discuss how this approach could be used to identify new hydrogen-bond patterns in situations in which biopolymers are encountered in unusual conditions, such as in non-aqueous mediums or at inorganic interfaces.

MM 39.3 Wed 15:30 H40
Invited Talk MM 39.3 Wed 15:30 H40
Competing oligonucleotide macromolecules: binding preferences instead of a ménage à trois — ●ALBRECHT OTT — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

The description of macromolecular recognition is usually reduced to the consideration of molecular pairs. In the simplest descriptions the receptor pairs exhibit a lock and key interaction, which mainly depends on the shape of the molecular recognizers, and this is supposed to lead to a highly specific recognition process. Much more refined and quantitative physical descriptions have been proposed, however, they are again based on pairwise interaction, and we remain far from understanding molecular binding in competition as it occurs in a biological organism. Here we present experiments on DNA macromolecular binding in competition. We identify situations where the binding constant of one DNA strand is highly dependent on the presence of another, very similar competitor. We interpret our findings as the result of an interaction term that leads to a formal equivalent of a Landau phase transition. We present experimental results from *in vitro* transcription assays that highlight the existence of other non-trivial competitive situations that may act along similar lines.

MM 39.4 Wed 16:00 H40
Poly(ethylene glycol) films and nanomembranes as flexible platform for humidity sensors and bioengineering — MUSAMMIR KHAN and ●MICHAEL ZHARNIKOV — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We discuss possible applications of novel poly(ethylene glycol) (PEG) hydrogel films and membranes (PHFs and PHMs). They were fabricated by thermally activated crosslinking of amine- and epoxy-terminated, star-branched PEG oligomers and characterized by tunable thicknesses of 4 - 200 nm. As demonstrated, PHFs and PHMs can be used as highly sensitive elements in humidity sensors and moisture-responsive nanoelectronic devices, relying on resistive transduction technique. Their resistance change by ca. 5.5 orders of the magnitude upon relative humidity variation from 0 to 100%, which is unprecedented response for homogeneous materials. As another representative example, we show that PHFs and PHMs are able to host protein-specific receptors, providing, at the same time, protein-repelling and humidity-responsive matrix with a characteristic mesh size up to 8.4 nm. A noticeable grafting density of the test avidin

protein, specifically attached to the biotin moieties coupled to the free amine groups in the PHMs, was achieved, whereas the analogous values for non-specifically adsorbed proteins were lower by a factor of 4-5. The engineering of PHMs with biomolecule-specific receptors and their loading with biomolecules are of potential interest for sensor fabrication and biomedical applications, including tissue engineering and regenerative therapy.

MM 39.5 Wed 16:15 H40

Dynamic biointerfaces: new generation of cell instructive materials — ●CHIARA FEDELE, RAVICHANDRAN H. KOLLARIGOWDA, SILVIA CAVALLI, and PAOLO A. NETTI — Center for Advanced Biomaterials for Healthcare, Istituto Italiano di Tecnologia, Naples, Italy

Nowadays the growing interest in tissue engineering and biology for the in vitro control of cell fate has led to the design of dynamically actuable platforms through the implementation of stimuli-responsive materials in order to mimic the continuous remodeling of the extracellular matrix in living systems. Dynamic biointerfaces are conceived in order to be able to modify in a predictable spatiotemporal manner the cell-material crosstalk, overcoming the limitations of static conventional biomaterials. In our work, azobenzene-containing photosensitive polymers (e. g. polymer brushes, thin films, crosslinked free standing polymers) are designed as biomaterials to obtain patterned or reshaping substrates using photolithographic techniques or single laser beam instruments, in some cases even in presence of cells, allowing for a real-time modification of cell behavior.

15 min. break

MM 39.6 Wed 16:45 H40

Tuning the Morphology of Langmuir Polymer Films through Controlled Relaxations of Non-Equilibrium States — ●RENATE REITER, SIVASURENDRAN CHANDRAN, and GÜNTER REITER — University of Freiburg, Experimental Polymer Physics, Freiburg, Germany

In general it is difficult to reproduce well defined morphologies of Langmuir polymer films (LPFs) because they have a high propensity to form non-equilibrium states. When these films are allowed to relax, a decay of the surface pressure with time might be observed indicating that the system is not equilibrated. Monitoring the temporal evolution of these relaxations and correlating them with snapshots of the corresponding morphologies sheds light on the associated structural reorganisation processes.

We present a systematic study based on different compression protocols designed to allow for relaxations of LPFs under well defined conditions. The homo peptide poly- γ -benzyl-L-glutamate (PBLG) was chosen for this study because it is a well investigated system that represents the relaxational behaviour of rod-like molecules which is expected to show less complexity than coiled polymer molecules. Our results demonstrate that experimentally manipulating the course of relaxations in LPFs has tremendous impact on the ordering of the molecules. Therefore various macroscopic properties of these biological relevant thin films are accessible.

MM 39.7 Wed 17:00 H40

Impact of Silver Nanoparticles on the mechanical properties of Aquabacterium biofilms — ●YVONNE SCHMITT¹, ALEXANDRA GRÜN¹, DIMITRI DEMESKO², WERNER MANZ¹, and SILKE RATHGEBER^{1,2} — ¹Institute for Natural Sciences, University of Koblenz-Landau, Koblenz, Germany. — ²Technology Institute for Functional Polymers and Surfaces (tifko) GmbH, Neuwied, Germany.

The antimicrobial properties of silver nanoparticles (AgNP) led to a wide range of applications in consumer products. As a consequence, there is an increasing release of AgNP into aquatic environments. Biofilms, a conglomerate of extracellular DNA, polysaccharides and proteins, play an important role in sediment stabilization in riverine systems. AgNP are supposed to be a continuous source for silver ions (Ag⁺) which can bind to functional groups of the biofilm constituents. This might lead to a decrease in the number of possible intermolecular interactions and, thus, reduced stability of the network. An impairment of the sediment stabilization due to enrichment of the AgNP in the biofilms might be detrimental to the whole ecosystem. In this work we studied the mechanical properties of an *A. citratiphilum* biofilm by means of rheology. The bacterium chosen is representative for a numerically dominant group of bacteria in different freshwater habitats. The biofilm was exposed to environmentally relevant concentrations of AgNP. In order to distinguish physical effects, resulting from the pres-

ence of the nanoparticles in the biofilms, from chemical effects, due to the activity of Ag⁺, we studied biofilms exposed to Ag⁺ as reference. We discuss our results in respect to their environmental implications.

MM 39.8 Wed 17:15 H40

Characterization of the behaviour of amino acids at bioactive calcite interfaces — ●ROBERT STEPIĆ¹, ZLATKO BRKLJAČA^{1,2}, DAVID M. SMITH^{2,3}, and ANA-SUNČANA SMITH^{1,2} — ¹Institute for Theoretical Physics and Excellence Cluster: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Nögelsbachstraße 49b, Erlangen, 91052, Germany — ²Rudjer Bošković Institute, Bijenička 54, 10000, Zagreb, Croatia — ³Center for Computational Chemistry, FAU Erlangen-Nürnberg, Nögelsbachstraße 25, Erlangen, 91052, Germany

The process of crystal growth controlled by biomolecules is known as biomineralization. This type of controlled growth results in crystals with a myriad of interesting properties, useful in a variety of applications. Therefore it is of great importance to gain deeper insights into the mechanistic details of interactions on the bioinorganic interface. For this purpose we present a systematic study of a set of amino acids, the elementary building blocks of peptides and proteins. Our methodology includes fully atomistic molecular dynamics simulations of the interface made of amino acids, water and slabs of calcite. Two different calcite slabs were taken into account, one with the stable (104) face and one with the unstable (001) face, which is associated with crystal growth. Free energies of binding to both surfaces for all the individual amino acids were determined using a series of sampling simulations with biasing potentials. These in turn reveal the importance of charged and polar groups in the interaction with calcite. This work provides reference data which can be helpful in further theoretical and experimental studies of calcite/peptide interfaces.

MM 39.9 Wed 17:30 H40

Biomimetic Surface Templating of Silica Nanoparticles by Lysine-Leucine Peptide on Au Substrate — ●HAO LU¹, YENENEH YIMER², RÜDIGER BERGER¹, MISCHA BONN¹, JIM PFAENDTNER², and TOBIAS WEIDNER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Chemical Engineering University of Washington, Seattle, USA

Fabrication of silica thin films and architectures has led to many applications in electronic and optical devices, cosmetics, and catalysis; recently, bioinspired silica fabrication approaches have attracted great attention because of low production cost and mild, sustainable fabrication methods. We are the first to demonstrate that the biomimetic molecules can also exert control over silica mineralization when bounded to inorganic surfaces. We use amphiphilic helical peptides based on leucine and lysine side chains (LK_a14) carrying cysteine terminal groups as linkers, providing stable covalent bond to gold surfaces. Using XPS, VSFG, and AFM, complemented by molecular dynamic simulation, we have investigated the silica mineralization process at the molecular level directly at the surface: In analogy to solution mineralization, the LK_a14 peptides on Au tend to assemble into ordered lateral structures, maintain their solution state helical folding and are oriented upright on the surface. The LK_a14 peptides nucleate silica nanoparticles at the surface, which then grow into larger, globular structures. This surface mineralization process serves as a well defined model system for lateral protein assembly and biomineralization and is of potential interest for the design of silica-based biomimetic coatings.

MM 39.10 Wed 17:45 H40

Reaction kinetics and diffusion in cell-free protein synthesis altered in polymer hydrogels — ●JULIAN THIELE¹, MAIKE M. K. HANSEN², DAVID FOSCHEPOTH², HANS A. HEUS², and WILHELM T. S. HUCK² — ¹Leibniz Institute of Polymer Research Dresden (IPF), Leibniz Research Cluster (LRC) and Department of Nanostructured Materials, Hohe Straße 6, 01069 Dresden, Germany — ²Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, NL

Despite the viscous and highly crowded interior of a cell and its influence on diffusion and reaction kinetics, in vitro studies on protein synthesis often fail to take into account the density and spatial organization of the cytoplasm.

We mimic the complex cellular environment using a porous hydrogel matrix, and study the effects of macromolecular crowding on gene expression. While gene expression is strongly decreased by macromolecular crowding in conventional dilute bulk solutions, both gene transcription and translation are significantly enhanced 5x and 4x, respectively, when performed in a microscopic hydrogel environment.

These results highlight the need to consider the influence of the physical environment on complex biochemical reactions including macromolecular crowding as well as microscale confinement and spatial organization.

MM 39.11 Wed 18:00 H40

Protein-protein interactions in crowded lysozyme solutions — ●KARIN JULIUS¹, MICHAEL PAULUS¹, JULIAN SCHULZE¹, STEFANIE ROESE¹, METIN TOLAN¹, and ROLAND WINTER² — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund — ²Fakultät Chemie, Technische Universität Dortmund, 44221 Dortmund, Germany

Inside cells, proteins are surrounded by different macromolecules, including proteins themselves, which cover approximately 30% of the

available volume. It has been shown that this reduction of free space by macromolecules, the so called crowding effect, has a significant impact on the stability of proteins, rendering them more resistant to temperature or pressure denaturation. However, the influence of crowding on the protein-protein interaction potential that is mediated by the solvent is still unknown. The final goal of this project is the investigation of the pressure dependent interaction potential between proteins in aqueous protein solution as a function of the crowder concentration, mimicking intracellular solution conditions. For this purpose, small-angle x-ray scattering (SAXS) under high hydrostatic pressure will be applied. As we will focus on the effect of crowding, the well characterized model protein lysozyme is used at a concentration of 5 - 10 wt.-% in combination with the macromolecular crowder Ficoll PM 70 and its monomeric subunit sucrose.

MM 40: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science IV - Atomic structure and defects III

Time: Wednesday 15:45–18:00

Location: H38

Topical Talk

MM 40.1 Wed 15:45 H38

Mapping local transient strain fields during in situ TEM deformation — ●CHRISTOPH GAMMER — University of Vienna, Physics of Nanostructured Materials — NCEM, Molecular Foundry, Lawrence Berkeley National Laboratory

While in situ TEM has provided insight into fundamental deformation mechanisms, the local strain during plastic deformation is of great importance to correlate defect structure with material properties.

In the present work we show that strain mapping can be carried out during continuous in situ deformation in a TEM at the nanometer scale. Two different types of tests are demonstrated. In the case of crystalline samples, our method is based on STEM diffraction mapping [1,2]. A direct electron detector is used to acquire diffraction patterns at a faster rate. Time resolved strain maps recorded during in situ deformation of an Al sample allow to measure local and transient strains occurring around moving dislocations. In addition an amorphous metallic glass sample was deformed in tension. For this experiment digital image correlation of decorated samples was used to obtain the time dependent local strain map revealing extreme localization of the deformation.

1. C. Gammer et al., Ultramicroscopy 155 (2015) 1.

2. V.B. Ozdol et al., Appl. Phys. Lett. 106 (2015) 253107.

We acknowledge support by the Austrian FWF [J3397] and the Molecular Foundry, U.S. Dept. of Energy, Contract #DE-AC02-05CH11231.

MM 40.2 Wed 16:15 H38

In-situ TEM isothermal annealing of nano-crystalline super-saturated Cu-Cr thin film alloys — ●TRISTAN HARZER, JAZMIN DUARTE, and GERHARD DEHM — Max-Planck-Institut für Eisenforschung GmbH, Structure and Nano-/Micromechanics of Materials, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany

The thermal stability and decomposition behavior of nano-crystalline single-phase Cu-Cr thin film alloys grown far from equilibrium were investigated by isothermal heat treatments. In the as-deposited state, the alloy films exhibit supersaturated solid solutions with a fcc and bcc structure for alloy compositions containing 4 at.% and 33 at.% Cr, respectively. Isothermal annealing in a temperature range of 150 °C - 500 °C were conducted inside a TEM and compared to phase stability data obtained by XRD under comparable annealing conditions. It is shown that the single phase nature of the alloy films is maintained for annealing temperatures of up to 300 °C, whereas heat treatment at temperatures of 400 °C or higher results in the formation of the two phase equilibrium film structures. Film decomposition in case of the Cu-4 at.% Cr thin film alloy proceeds via enrichment of Cr at grain boundaries and grain boundary diffusion whereas phase separation of the Cu-33 at.% Cr thin film alloy progresses predominantly via volume diffusion. Temperature dependent diffusion coefficients for volume and grain boundary diffusion along with the respective activation energies are determined from analytical in-situ TEM. In addition, the influence of electron beam irradiation on the diffusion kinetics is considered.

MM 40.3 Wed 16:30 H38

Assessing phase stability and element distribution in Co-base superalloys at elevated temperatures by in situ TEM heating

experiments. — ●YOLITA EGGELER, JULIAN MÜLLER, and ERDMANN SPIECKER — Lehrstuhl für Mikro- und Nanostrukturforschung & Center for Nanoanalysis and Electron Microscopy (CENEM), Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg, Cauerstraße 6, 91058 Erlangen

Co-based alloys, of a composition of Co-12Al-9W, form a stable two phase γ/γ' microstructure at 900 °C [1]. γ' cubes, consisting of the L12 crystal structure are coherently embedded in a solid solution fcc (A1) γ matrix. To ensure precipitate hardening at temperatures, which are relevant to practical applications, 700-1100 °C, as experienced in gas turbine applications, the stability of the γ/γ' phases is of fundamental importance. In this analysis in situ TEM studies with chip-based heating systems (by DENS solution) are applied on new Co-based superalloys. After in situ heating at apr. 900 °C and controlled quenching with different quenching rates the elemental distribution at the γ/γ' interface is measured using ChemiSTEM EDX. Exploiting the driving force for interface movement resulting from temperature-dependent volume fraction of γ and γ' insight into the diffusion of individual alloying elements and the relationship between local chemistry and ordering can be gained from transient phenomena. The experimental results will be compared with theoretical calculations. This work has been carried out within the framework of the SFB-TR 103 "Single Crystal Superalloys". [1] J. Sato et al, Science (2006), vol.312, p. 90

15 min. coffee break

MM 40.4 Wed 17:00 H38

Nanostructured Metallic Glasses: Tailoring the Mechanical Properties of Amorphous Metals — ●KARSTEN ALBE, TOBIAS BRINK, and OMAR ADJAOUD — TU Darmstadt, Fachbereich Material -und Geowissenschaften, FG Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt

The mechanical properties of metallic glasses can not only be influenced by their chemical composition, but also by their nanostructure: Secondary phases in the form of precipitates, as well as a glass-glass interfaces are possible means to enhance the plasticity of the material. In this contribution results from molecular dynamics simulations of nanostructured Cu-Zr based metallic glasses under external load will be discussed and compared with experimental findings, especially with results from transmission electron microscopy. The influence of crystalline nanoprecipitates on shear band nucleation and propagation is investigated, and also the effect of grain size and composition on the deformation behavior of nanoglasses and nanoglass composites.

MM 40.5 Wed 17:30 H38

Medium range order in Pd-based glasses — ●VITALIJ SCHMIDT¹, HARALD RÖSNER¹, MARTIN PETERLECHNER¹, GERHARD WILDE¹, and PAUL VAYLES² — ¹Institut für Materialphysik, Universität Münster — ²Materials Science and Engineering, University of Wisconsin-Madison

Metallic glasses exhibit superior mechanical properties like high yield strength or wear and corrosion resistance. However after a large elastic regime they are prone to catastrophic failure especially under tensile load. This motivates an interest in understanding the deformation

behavior of metallic glasses. Deformation tests on metallic glasses performed well below the glass transition temperature have shown that the plastic flow is restricted to narrow regions called shear bands. They are associated with a structural changes (free volume) compared to the surrounding matrix due to shear localization. Thus modifications of the local short or medium range order (SRO, MRO) are expected in shear bands.

In order to study directly the structural changes fluctuation electron microscopy (FEM) has been used to characterize Pd-based metallic glass samples by analyzing sets of nanobeam diffraction patterns (NBDPs). The variance of the individual patterns were extracted from azimuthal profiles and normed by the mean intensity squared. This way a directly comparable normalized variance is obtained. Samples of different states (as-cast, deformed, annealed) and chemical compositions (micro-alloying) are compared.

MM 40.6 Wed 17:45 H38

Analysis of local atomic arrangement in layered Ge-Sb-Te crystal structures by advanced scanning transmission electron microscopy — ●ANDRIY LOTNYK, ULRICH ROSS, SABINE BERNÜTZ, ERIK THELANDER, and BERND RAUSCHENBACH — Leib-

niz Institute of Surface Modification (IOM), Permoserstr. 15, D-04318 Leipzig, Germany

The knowledge on the proper local atomic arrangement in Ge-Sb-Te compounds is of particular interest for optical and electronic applications such as data storage, thermoelectric and ferroelectric. In this work, we study the local atomic arrangements in Ge-Sb-Te thin films consisting of layered $\text{Ge}_2\text{Sb}_2\text{Te}_5$, $\text{Ge}_1\text{Sb}_2\text{Te}_4$ and $\text{Ge}_3\text{Sb}_2\text{Te}_6$ crystal structures by using state of the art atomic-resolution aberration-corrected (Cs-corrected) high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and proper theoretical image simulations. The results show that the intensities in simulated Cs-corrected HAADF-STEM micrographs are very sensitive to thermal displacement factors in the studied structures at specific lattice sites. Based on these findings, we are able to determine proper stacking sequences in the Ge-Sb-Te phases by comprehensive analyses of experimental and simulated image intensities. The experimental data reveal that the Ge and Sb atomic species tend to form intermixed cation layers which differ from theoretical predictions. However, the ratio of Sb to Ge is different in distinct cation layers. The obtained data are discussed with respect to existing experimental and theoretical structure models reported for bulk Ge-Sb-Te materials.

MM 41: Methods in Computational Materials Modelling I: Ab initio thermodynamics

Time: Wednesday 15:45–18:00

Location: H52

MM 41.1 Wed 15:45 H52

High-pressure phases of Li-S binaries — ●LILIA BOERI, CHRISTIAN KOKAIL, and CHRISTOPH HEIL — Institute for Theoretical and Computational Physics, Graz University of Technology, Graz (Austria)

Together with hydrides, high-pressure phases of Li-rich solids are natural candidates to for high- T_c conventional superconductivity [1] and other quantum effects. [2] In this study we use methods for ab-initio crystal structure prediction [3] to study the phase diagram of the binary system Li-S, i.e. the lithium analog of the record conventional superconductor H3S.[4]

We show that several compositions which are not stable at ambient pressures are stabilized at high pressures; similarly to other Li binaries, some of these phases display semiconducting-to-metal and semiconducting-to-superconductor phase transitions. [5]

[1] N. W. Ashcroft, Phys. Rev. Lett. **92**, 187002 (2004). [2] J. B. Neaton and N.W. Ashcroft, Nature **400**, 141 (1999). [3] A. P. Drozdov, et al Nature **525**, 73 (2015); D. Duan, et al, Sci. Rep. **4** 6968 (2014). [3] A. R. Oganov and C.W. Glass, J. Chem. Phys. **124**, 244704 (2006). [5] Y. Xie et al., Phys. Rev. Lett. **104**, 177005 (2010); Y. Shen et al., arXiv 1504.06677 (2015).

MM 41.2 Wed 16:00 H52

Ab initio description of phase transitions in pure Ti at finite temperatures — ●DOMINIQUE KORBMACHER, ALBERT GLENSK, BLAZEJ GRABOWSKI, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti and its alloys play an important role in many industrial applications, for example in medicine or aircrafts. In this project we investigate pure Ti within a fully *ab initio* based methodology using density-functional theory and including anharmonicity. Because bcc Ti is dynamically unstable at lower temperatures standard approaches cannot be applied. We have therefore developed a new method (referred to as TU-TILD [1]) which allows to capture the anharmonic contribution also for unstable systems. This method is based on optimized interatomic potentials which can be used as a highly efficient reference for thermodynamic integration. Applying the TU-TILD methodology, we have accurately investigated the phase stabilities of the three relevant phases in Ti (ω , hcp and bcc). In particular we calculated the free energies and derived thermodynamic properties for the whole temperature regime up to the melting point, using two different exchange-correlation functionals. We show that the ω to hcp as well as the hcp to bcc phase transition are correctly predicted by our methods. Furthermore we discuss the second order bcc to ω phase transition.

[1] A. I. Duff, et al., PRB **91**, 214311 (2015).

MM 41.3 Wed 16:15 H52

Including DFT data in phase diagram calculations for zirconium carbide — ●THERESA DAVEY¹, ANDREW DUFF¹, SUZANA

FRIES², and MICHAEL FINNIS^{1,3} — ¹Department of Materials, Imperial College London, London SW7 2AZ, UK — ²ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — ³Department of Physics, The Thomas Young Centre, Imperial College London, London SW7 2AZ, UK

The CALPHAD approach takes experimental data and parameterises Gibbs energy curves with an optimal fit to this data, which can be phase boundary measurements or thermodynamic data. Thermo-Calc, and other phase diagram assessment codes, make no reference to the vacancy formation energy explicitly, leaving it only to be referred to implicitly within the Gibbs energy formulation [1]. Nevertheless, vacancy formation energies must significantly affect the phase stability when compounds are not strictly stoichiometric.

In recent years, theoretical calculations of the vacancy formation energy (or other point defect formation energies), which are difficult or impossible to measure experimentally, have been produced. This data could be used to increase the physical information encoded within a thermodynamic database.

For the zirconium-carbon phase diagram, I show how data from DFT calculations of the vacancy formation energy in the zirconium carbide phase can introduced as a constraint on the parameterisation of the Gibbs energy, and how this changes the resulting phase diagram.

[1] J. Rogal et al. (2014), Phys. Status Solidi B, 251(1) 97-129.

MM 41.4 Wed 16:30 H52

Formation Energy of Ions in Water using ab-initio Molecular Dynamics — ●ANOOP KISHORE VATTI, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Understanding hydration of ions is key feature for chemical and biological processes occurring in water and the specific adsorption of ions at solid-liquid interfaces. Identification of theoretical concepts that allow to probe accurately and computationally efficiently reproduce the complex atomic and electronic structure of ions in liquid water at the microscopic level is crucial. We performed an extensive ab-initio molecular dynamics simulations to study the solvation of charged and neutral cations (Zn/Mg)/anions(Cl/Br/I) in water. Structural correlations and electronic properties of the studied ions are analyzed and compared to experimental observations. Method used here for the calculation of formation energies is inspired from the semiconductor defect chemistry approach. Aligning the water band edges on an absolute scale allows us to benchmark calculated formation energies and transition states, and compare them to experiment[1]. We find a good agreement with photo-emission experiments[2] for the calculated transition levels for the anions in water.

[1] M. Todorova and J. Neugebauer, Phys. Rev. Applied 1, 014001 (2014).

[2] B. Winter et al., JACS 127, 7203 (2005).

15 min. coffee break

MM 41.5 Wed 17:00 H52

Intricacies of phonon line shapes in random alloys: A first-principles study — ●BISWANATH DUTTA¹, DEBASHISH DAS², SUBHRADIP GHOSH², BIPLAB SANYAL³, TILMANN HICKEL¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — ²Department of Physics, IIT Guwahati, Guwahati 781039, India — ³Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Lattice vibrations in random alloys are governed by the amount of mass and force-constant disorder present in the system. Disorder-induced scattering in these systems results in broadening of phonon peaks, which can be asymmetric and (for extreme disorder) can even split into two branches. To calculate phonon frequencies, lifetimes, as well as the complex phonon line shapes, sophisticated modeling approaches are required. We use the itinerant coherent potential approximation (ICPA), a Green's function based formalism to account for local fluctuations in random alloys. The interatomic force-constants are calculated using density functional theory and are fed into ICPA to perform the configuration averaging. Our computed results for Cu-Au and Ni-Pt alloys show that a single Lorentzian function cannot describe the phonon line shapes for several wave-vectors. The comparison between theory and experiment also depends on the choice of the Lorentzian function. We discuss the results in the framework of phonon line shape convolution and conclude that multiple Lorentzian fitting for certain wave-vectors in random alloys gives new insights on phonon frequencies and their line widths which can be relevant for their functional properties.

MM 41.6 Wed 17:15 H52

The effects of lattice vibrations on electronic and magnetic properties of paramagnetic Fe: A disordered local moments molecular dynamics study — ●BJÖRN ALLING — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf — Linköping University, Sweden

High temperature lattice vibrations in the paramagnetic states of Fe is studied employing the disordered local moments molecular dynamics (DLM-MD) method. In particular its impact on the magnetic and electronic structure is investigated. It is found that lattice vibrations strongly affect the local magnetic moment distribution which correlates with the local atomic volumes. Without explicit vibrations, the mean local magnetic moment and mean field derived magnetic entropy in paramagnetic bcc Fe are larger in comparison to paramagnetic fcc Fe which would indicate that magnetic degree of freedom contribute to stabilize the bcc phase at high temperatures. However, when explicit lattice vibrations are taken into consideration, the picture is changing at high temperature and very similar local magnetic moment distributions and mean-field magnetic entropies of bcc and fcc Fe are found close to the γ to δ transition. This qualitative change, due to vibrations, is consistently observed in the electronic density of states which are found to become equally similar with increasing temperature. Our findings illustrate the need for an explicit consideration of vibrational

disorder and its impact on electronic and magnetic properties to understand paramagnetic Fe.

MM 41.7 Wed 17:30 H52

Electron-phonon interactions in 2D materials: going beyond the limitations of plane-wave density-functional theory — ●THIBAUT SOHIER^{1,2}, MATTEO CALANDRA², and FRANCESCO MAURI^{2,3} — ¹THEOS and NCCR MARVEL, EPFL, Switzerland — ²IMPMC, Sorbonnes Universités, UPMC, UMR CNRS 7590, 4 place Jussieu, 75005 Paris, France — ³ISC-CNR and Dept of Physics, Sapienza University of Rome, P.le A. Moro 5, 00185, Rome, Italy

Electron-phonon interactions and their role in the transport properties of 2D materials are conceptual milestones for tomorrow's nanoelectronics. Electron-phonon interactions depend strongly on dimensionality, especially when long-range Coulomb interactions are involved, as in screened couplings or the coupling to polar optical phonons.

A key limitation of plane-wave density-functional perturbation theory with local functionals for the simulation of 2D materials is the use of periodic boundary conditions, implying the presence of periodic images of the 2D system in the out-of-plane direction. Long-range Coulomb interactions between those periodic images lead to incorrect electron-phonon couplings in 2D materials such as graphene or MoS₂.

We develop novel approaches to eliminate the interactions between periodic images by truncating the Coulomb interaction in the out-of-plane direction. This is implemented for the calculation of total energy, forces, phonons and electron-phonon interactions, with possible addition of an asymmetric electric field to dope the 2D material. We use this method to investigate the peculiarity of the electron-phonon interaction in 2D materials like graphene and MoS₂.

MM 41.8 Wed 17:45 H52

Discovering complete pressure-temperature phase diagrams with Hamiltonian Monte Carlo nested sampling — ●ROBERT BALDOCK¹, NOAM BERNSTEIN², LIVIA PARTAY¹, MICHAEL PAYNE¹, and GABOR CSANYI¹ — ¹University of Cambridge, UK — ²Naval Research Laboratory, USA

Nested sampling is a Monte Carlo algorithm that can be used to efficiently calculate the complete configurational density of states in a material that undergoes multiple first-order phase transitions. From the density of states one can calculate the partition function as an explicit function of temperature and perform statistical mechanics from first principles. Indeed, we have shown how nested sampling can be used to automatically discover complete pressure-temperature phase diagrams with no prior knowledge of the locations of phase transitions or the structures of phases. In this talk I will present a new version of the nested sampling algorithm, based on a modified Hamiltonian ("Hybrid") Monte Carlo scheme. This new scheme reduces the scaling of a general nested sampling calculation. In particular the new algorithm expedites the sampling of atomic configuration spaces in condensed phases, and permits one to perform nested sampling calculations at a fraction of the cost required by ordinary nested sampling with standard Monte Carlo.

MM 42: Functional materials III: Actuators, sensors and functional devices

Time: Wednesday 15:45–17:30

Location: H53

MM 42.1 Wed 15:45 H53

Potential impurity dopants in molybdenum oxide — ●JULIANA SCHELL^{1,2}, CARLOS DÍAZ-GUERRA³, KATHARINA LORENZ⁴, and JOÃO GUILHERME MARTINS CORREIA^{1,5} — ¹Isotope Mass Separator On-Line ISOLDE, CERN, Switzerland — ²Universität des Saarlandes, Saarbrücken, Germany — ³Dpto. Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Spain — ⁴Instituto Superior Técnico, Universidade de Lisboa, Portugal — ⁵Centro de Ciências e Tecnologias Nucleares, Universidade de Lisboa, Portugal

Important technological applications, especially as a promising material for future electrochromic imaging devices have motivated the present work where we investigate at the atomic scale the introduction of potential dopants (Cd, Lu) in molybdenum oxide by ion implantation. Cd in MoO₃ is intended to be an electrical dopant and may improve the transport properties of these materials while rare

earth doping is investigated for their light emission characteristics. At ISOLDE-CERN Perturbed Angular Correlation Spectroscopy (PAC), has been used to study recovery of defects and the local situation of implanted 111mCd and 172Lu on single crystals as a function of annealing and measuring temperatures. The electric field gradients (EFG) show evidence for Cd or Lu occupying two regular sites on MoO₃. In the case of the Lu/Yb, most of the probe atoms interact with lattice or electronic defects. This might be related to irregular lattices sites, damaged environment or dynamic electronic effects resulting from the electronic recombination after decay of 172Lu.

MM 42.2 Wed 16:00 H53

Energiespeicherung in Textilien mit faserbasierten Batterien — ●MARINA NORMANN¹, ANNE SCHWARZ-PFEIFFER¹ und ANDREA EHRMANN² — ¹Niederrhein University of Applied Sciences, Faculty of Textile and Clothing Technology, Mönchengladbach (Germany) — ²Bielefeld University of Applied Sciences, Faculty of Engineering

Sciences and Mathematics, Bielefeld (Germany)

Im Bereich der "Smart Textiles", der intelligenten Textilien, werden herkömmliche textile Materialien mit neuen Funktionalitäten versehen. Die Integration elektronischer Bauteile in Textilien erlaubt es beispielsweise, neue Design-Effekte und Funktionen zu erzeugen oder Vitalfunktionen mit tragbaren Diagnosesystemen rund um die Uhr zu detektieren. Auch die Weiterentwicklung von Fasern zu Sensoren und Aktuatoren wird durch neue Materialien, wie leitfähige Polymere, möglich. Solche elektronischen Zusatzfunktionen erfordern jedoch eine adäquate Energieversorgung.

Hierzu wird in einem aktuellen Projekt eine textile Batterie entwickelt, in der verschiedene metallische und metallbeschichtete textile Strukturen als Elektroden dienen, die durch eine elektrolytgetränkte Vliesstruktur separiert werden. Auf diese Weise kann eine rein textile Lösung zur Energiespeicherung erzeugt werden, um vollständig faserbasierte "Smart Textiles" zu entwickeln. Die Kombination traditioneller textiler Prozesse mit leicht hochskalierbaren Technologien erlaubt es zudem, die Produktionskosten niedrig zu halten.

Der Vortrag zeigt aktuelle Forschungsergebnisse und gibt einen Ausblick auf die geplanten weiteren Forschungsansätze in dem Projekt.

MM 42.3 Wed 16:15 H53

High-pressure polymorphism as a step towards high density structures of LiAlH₄ — XIAOLI HUANG, DEFANG DUAN, FANGPEI LI, LU WANG, GANG WU, BINGBING LIU, and •TIAN CUI — State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun 130012, P. R. China

Ternary aluminum hydrides could be an extremely efficient energy storage system owing to their high gravimetric and volumetric hydrogen densities. Of these, LiAlH₄ is a prominent hydrogen-storage material with 10.6 wt% theoretical hydrogen content and thus has recently received much attention. The search for polymorphism with high volumetric hydrogen densities is a key resource for hydrogen storage materials. The great interest in high pressure phase transformations of LiAlH₄ has been aroused by a theoretical prediction of a new high pressure phase. However, the crystal structures as the key to understand the intriguing high pressure behavior of LiAlH₄ remained elusive for several decades. In order to clearly explore the behavior of LiAlH₄ under high pressure, we have investigated the high pressure structures of LiAlH₄ by a joint theoretical and experimental study. And we have uncovered two crystal structures (β -LiAlH₄ and γ -LiAlH₄) as metastable low-energy polymorphs, which are not reported in previous literatures. The first phase transition is accompanied by the local structure change from a distorted AlH₄ tetrahedron into a distorted AlH₆ octahedron, which contributes to a large volume collapse with 20%. This new structure may show completely different hydrogen storage properties if stabilized by chemical substitution at ambient pressure.

15 min. coffee break

MM 42.4 Wed 16:45 H53

Hydrogen-assisted actuation with nanoporous palladium — •SHAN SHI^{1,2}, JÜRGEN MARKMANN^{1,2}, and JÖRG WEISSMÜLLER^{1,2} — ¹Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — ²Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg

Nanoporous (np) metals made by electrochemical dealloying exhibit a three dimensional metal network with high specific surface area, which couples the entire material behaviour to surface effects and specifically to electrocapillary effects that induce stress in the network. While dealloying has been demonstrated for many transition metals, studies requiring homogeneous and monolithic np samples have remained restricted to nanoporous gold and gold-based alloys. Based on a sys-

tematic optimization of master alloy composition, electrolyte, as well as temperature and potential of corrosion we here demonstrate the preparation of mm-size homogeneous monolithic np palladium (Pd) samples. Thermal coarsening allows to adjust the characteristic ligament size between 30 and 300 nm. Pd readily dissolves hydrogen, which results in volume expansion. We explore the influence of electrocapillary coupling at the surface and of hydrogen alloying in the bulk on the effective macroscopic mechanical strain of np-Pd during electrochemical potential cycles. A remarkably large reversible strain amplitude (about 3.4%), fast response time, and good stability of our np-Pd actuator emphasizes the prospects of np-Pd as a novel functional material.

MM 42.5 Wed 17:00 H53

Surface stress charge response of nickel in alkaline solutions — •CHUAN CHENG and JÖRG WEISSMÜLLER — Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, 21073 Hamburg, Germany

Charge induced reversible strain was recently found in nanoporous structured nickel upon cyclic potential triggering in alkaline solutions [1,2]. Different from metallic actuators with clean metal surfaces, the surface of Ni is covered with several nanometers thick Ni(II) passive layer, which can cause reversible volume change during Ni(II)/Ni(III) redox reactions. The situation becomes even more complex as different types of Ni(II) can be formed on Ni surface, which exhibit opposite signed volume change when they are oxidized into Ni(III). In this work, surface stress charge response of Ni in alkaline solutions will be characterized by an in situ electrochemical cell. Ni thin film is sputtered on one side of a Si cantilever. Charge induced surface stress in Ni, which causes bending of the cantilever, was measured by a laser-based setup. The surface stress charge coefficients at both capacitive double layer region and the redox region are obtained. This work will provide a fundamental understanding of Ni based electrochemical actuators.

References:

1. M. Hakamada, S. Matsumura, and M. Mabuchi, Mater. Lett. 70, 132 (2012).
2. C. Cheng and A. H. W. Ngan, ACS Nano 9, 3984 (2015).

MM 42.6 Wed 17:15 H53

Tunneling current calculations across diamondoid-functionalized electrodes: impact on biosensing — GANESH SIVARAMAN¹, RODRIGO G. AMORIM², RALPH H. SCHEICHER³, and •MARIA FYTA¹ — ¹Institute for Computational Physics, University of Stuttgart, Germany — ²Departamento de Física, Universidade Federal Fluminense, RJ, Brazil — ³Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

Attaching specific molecules to a pair of opposing metal electrodes is known to enhance tunneling current signals measured across them. This functionalization of electrodes can make them more selective in sensing and detecting DNA molecules translocating between the electrode gap. Diamondoids are tiny hydrogen-terminated diamond-like cages which can be produced in a variety of sizes and can be selectively chemically modified, showing a high potential as functionalization units. Here, we focus on the quantum-transport properties of diamondoid-functionalized Au(111) break-junctions. For the functionalization, different diamondoids are considered and the tunneling current signals arising from different DNA units (the nucleobases) in the break-junction are investigated. We report on the read-out characteristics and the sensitivity of the functionalized electrodes to identify the four DNA nucleobases and their mutations. Such electrodes can be embedded in nanopores which are able to electrophoretically thread DNA. Our results indicate that a device based on diamondoid-functionalized electrodes could have a high potential in sequencing DNA with a strong impact in nanopore research and biosensing methodologies.

MM 43: Frontiers of Electronic-Structure Theory: Focus on Topology and Transport

Time: Wednesday 18:15–20:30

Location: Poster A

MM 43.1 Wed 18:15 Poster A

Improving anharmonic vibrational calculations from first principles — •JOSEPH C.A. PRENTICE, BARTOMEU MONSERRAT, and RICHARD J. NEEDS — TCM Group, Cavendish Laboratory, University of Cambridge, UK

The vibrational self-consistent field (VSCF) method, as described in PRB 87 144302, has had several successes in accurately calculating the anharmonic properties of various materials, such as diamond, ice and solid hydrogen. However, a practical issue with the method is the large number of DFT calculations required to map the Born-Oppenheimer energy surface sufficiently accurately. We look at improvements to the

method that reduce this computational load, in particular using data on forces from DFT calculations to improve the accuracy of the mapping. Results using this improved method are presented for competing structures of silicate perovskite under lower mantle conditions. Further improvements, involving the inclusion of n-body coupling between phonons, and their possible implementation are also discussed.

MM 43.2 Wed 18:15 Poster A

Towards a practical implementation of second-order Møller-Plesset perturbation theory for solids — •XIANGYUE LIU, ARVID CONRAD IHRIG, SERGEY LEVCHENKO, IGOR YING ZHANG, and MATTHIAS SCHEFFLER — *Fritz-Haber-Institut der MPG, Berlin, DE*

The second-order Møller-Plesset perturbation theory (MP2) method is gaining attention in materials science, because it is free from the one-electron self-interaction error. Such error, as a lasting problem in density-functional theory, can lead to a wrong prediction of electronic band gaps, charge transfers, and reaction barriers, all of which are ubiquitous electronic properties or behaviors in condensed-matter systems. However, the unfavourable computational complexity, especially the cubic scaling with respect to the k -point number in reciprocal space, limits the applicability of MP2 for solids. In this project we present a practical MP2 implementation for solids in the all-electron full-potential framework. In our implementation, the MP2 correlation energy is evaluated in the atomic-orbital (AO) representation (AO-MP2), which allows for a lower computational scaling in both real and reciprocal spaces[1]. The localized resolution of identity (RI-LV) technique[2] is adopted to address the memory bottleneck of the AO-MP2 method, making it feasible to handle systems with several hundred atoms per supercell while avoiding the reliance on the disk storage. We demonstrate the accuracy as well as the efficiency of our new MP2 implementation for a diverse set of materials. [1] Levchenko, S. V. *et al.*, *Comput. Phys. Comm.* **192**, 60, (2015); [2] Ihrig, A.C. *et al.*, *New J. Phys.* **17** 093020, (2015).

MM 43.3 Wed 18:15 Poster A

Application of the exact exchange functional to magnetic metals within the FLAPW method — •MAX NUSSPICKEL¹, MARKUS BETZINGER¹, CHRISTOPH FRIEDRICH¹, ANDREAS GÖRLING², and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — ²Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Orbital-dependent functionals form a promising class of exchange-correlation (xc) functionals in Kohn-Sham density-functional theory. Already the simplest functional of its kind, the exact exchange functional (EXX), cures the unphysical Coulomb self-interaction error of LDA and GGA functionals. In order to obtain a local xc potential from an orbital-dependent functional, the optimized effective potential (OEP) method is used, resulting in an integral equation for the potential. This equation, however, determines the potential only up to a constant.

In spin-polarized metals, the alignment of the spin-up and spin-down potentials is obtained by the requirement of electron number conservation: variations of the potential can lead to a change of the Fermi energy and, hence, to a variation of the densities of both electron spins. In this way, the OEP equations for the spin-up and spin-down potentials are coupled and the spin-dependent xc potential is obtained from a single OEP equation. We discuss the extension of our EXX-OEP implementation within the linearized augmented plane-wave (FLAPW) method and show results for prototype magnetic metals.

MM 43.4 Wed 18:15 Poster A

Electric switchable giant Rashba-type spin splitting in bulk PbS — •BIN SHAO¹, WENHUI DUAN², and THOMAS FRAUENHEIM¹ — ¹BCCMS, University of Bremen, Bremen, Germany — ²Institute for Advanced Study, Tsinghua University, Beijing, China

Realizing electric controllable spin is one of the major challenges in the field of spintronics. A promising approach is to utilize so-called Rashba effect, which arises from the spin-orbit coupling under broken inversion symmetry, leading to a momentum-dependent spin splitting in k -space. However, the sizes of this splitting are usually rather small, which hinders the application of this effect in spintronics. In this work, based on density functional calculation, we predict a giant Rashba-type spin splitting in bulk PbS with space group $P6_3mc$. The phonon spectrum calculation gives evidence of the thermal stability of this system. The origin of the giant Rashba effect has been demonstrated from the deviation of the S ion from the inversion symmetric position, leading

to an ferroelectric polarization along c axis. By switching the direction of the ferroelectric polarization, the spin directions of bulk carriers governed by the Rashba effect are completely rotated, which grants a potential approach to manipulate the spin of electrons by an external electric field. Moreover, under a reasonable hydrostatic pressure, the system could obtain the inversion symmetry due to the movement of the S ion backwards to symmetric positions. As a result, the system turns into a topological phase with the massless Dirac cone state at the (001) surface.

MM 43.5 Wed 18:15 Poster A

GW+ fRG : Towards an fRG enhancement of *ab initio* calculations — JANNIS EHRLICH^{1,2}, CARSTEN HONERKAMP¹, CHRISTOPH FRIEDRICH², and •STEPHAN BLÜGEL² — ¹Institut für theoretische Festkörperphysik, RWTH Aachen University, D-52056 Aachen, Germany — ²PGI-1 and IAS-1, FZJ & JARA, D-52425 Jülich, Germany

Spin excitations in solids are of fundamental interest for a wide variety of phenomena. Most materials-specific theoretical studies are based on the adiabatic treatment of the spin-degrees of freedom in the context of DFT. Approaches based on the GW approximation include screening effects due to charge fluctuations but neglect vertex corrections and other contributions like magnetic fluctuations. The functional renormalization group (fRG) can overcome these limitations as it resums a different class of diagrams, among them charge and magnetic fluctuations and vertex corrections. We discuss how the equations for two-particle vertices in the fRG contain the GW approximation, the Bethe-Salpeter equation (BSE) and the parquet approach on certain levels of approximations. Thus, a fRG calculation of materials properties could be a powerful approach to improve the GW and BSE methods already applied in first-principles calculations. By using recently suggested channel decomposition schemes [1,2] the method has gained in flexibility and in potential for tackling more complex tasks. Here we propose first steps to develop the fRG approach for the *ab initio* calculation of materials properties.

- [1] C. Husemann, M. Salmhofer, *Phys. Rev. B* **79**, 195125 (2009).
[2] W. Wang *et al.*, *Phys. Rev. B* **85**, 035414 (2012).

MM 43.6 Wed 18:15 Poster A

The quantum anomalous Hall effect in HgMnTe — •JAN BÖTTCHER, CHRISTOPH KLEINER, and EWELINA M. HANKIEWICZ — Uni Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Recently, the quantum anomalous Hall (QAH) effect was predicted to exist in Mn doped HgTe . Within the QAH phase only one edge state remains at an edge due to an opposite coupling of spin to the magnetization. The experimental proof is however still outstanding. The paramagnetic nature of the Mn impurities gives rise to the formation of Landau levels which makes it experimentally challenging to distinguish the QAH from a conventional quantum Hall (QH) state. Based on the BHZ model, we present an extended study of the transition from the quantum spin Hall to the QAH state as well as the QAH to the quantum Hall state. For this purpose, we make use of the finite difference method and compare the results with analytical calculations. Hallmarks of the QAH states in the presence of magnetic fields are discussed. The BHZ model has natural limitations in the high magnetic field regime. We therefore compare our results with band structure calculations based on the 8×8 Kane Hamiltonian. Signatures in the magnetoresistance are discussed which might open the door to distinguish the QAH from the QH state in future transport experiments.

We acknowledge financial support by the DFG within SFB 1170 "ToCoTronics".

MM 43.7 Wed 18:15 Poster A

Nonconventional screening of the Coulomb interaction in low-dimensional semiconductors and insulators — ERSOY SASIOGLU, •CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Screening effects play a fundamental role in determining the exciton binding energy, electron dynamics, and the effective electron-electron interaction in low-dimensional semiconductors and insulators. Experimental observation of the large exciton binding energies and nonhydrogenic Rydberg series in low-dimensional semiconductors indicate an unusual non-local screening of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation (RPA) within the FLAPW method we study the screen-

ing of the Coulomb interaction in low-dimensional semiconductors and insulators. For this purpose a novel tetrahedron method has been implemented. We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the screened interaction W cannot be expressed by a simple static dielectric constant. We compare the numerical RPA results to analytical functions derived from image-

charge models for the isolated slab and for a repeated slab model. We find a nonconventional screening in low-dimensions. This nonconventional screening explains the deviations from the usual hydrogenic Rydberg series of energy levels of the excitonic states in one- and two-dimensional semiconductors and opens up possibilities for fundamental studies of correlation effects in low-dimensional materials.

MM 44: Invited talk Sandloebes

Time: Wednesday 18:30–19:00

Location: H38

Invited Talk

MM 44.1 Wed 18:30 H38

Design of ductile Mg alloys based on combined high resolution electron microscopy experiments and ab initio calculations — ●STEFANIE SANDLÖBES^{1,2}, MARTIN FRIÁK^{1,3}, ZONGRUI PEI¹, TALAL AL-SAMMAN², SANDRA KORTE-KERZEL², JÖRG NEUGEBAUER¹, and DIERK RAABE¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany — ³Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

Single phase solid solution Mg-Y shows an increase in room temperature ductility by about 5 times compared to pure Mg, while maintaining comparable strength and enabling stable work hardening. We show

that the enhancement of the mechanical properties of Mg-Y alloys is caused by facilitated activation of additional deformation mechanisms providing a $\langle c \rangle$ -dislocation shear component. By employing complementary high-resolution electron characterization methods and ab initio calculations we identified the I1 stacking fault energy (SFE) as a guiding parameter for ductility in Mg alloys. Using the parameter SFE I1 we performed ab initio calculations and identified further favourable solid solution elements, rendered into both, binary and ternary alloys, which decrease the SFE I1 in Mg and, indeed, show increased room temperature ductility. We demonstrate that combining ab initio and advanced experimental characterization methods facilitates the identification and understanding of critical alloying and associated microstructure parameters as basis for advanced alloy design.

MM 45: Invited talk Horbach

Time: Wednesday 19:00–19:30

Location: H38

Invited Talk

MM 45.1 Wed 19:00 H38

Computer simulation of bulk-metallic glasses under shear: From inhomogeneous flow patterns to mechanical properties — ●JUERGEN HORBACH¹, GAURAV PRAKASH SHRIVASTAV¹, and PINAKI CHAUDHURI² — ¹Institute for Theoretical Physics II, University of Düsseldorf, Germany — ²The Institute of Mathematical Sciences, Chennai, India

The response of glasses to mechanical loading often leads to the formation of inhomogeneous flow patterns that may strongly affect the materials properties. Among them, shear bands, associated with strain

localization in form of band-like structures, are ubiquitous in a wide variety of materials, ranging from soft matter systems to metallic alloys. Molecular dynamics simulations of a model of Ni₈₀P₂₀ are performed to investigate the formation of shear bands, using different flow protocols. Under an externally applied constant stress, persistent creep in the form of shear-banded structures is observed around the yield stress, whereas under the application of a constant strain rate, shear bands occur at sufficiently low strain rates. We analyze the nucleation of the shear-banded structures as well as the mechanical properties of the deformed glasses.

MM 46: Annual General Assembly of the MM Division

Time: Wednesday 19:45–20:45

Location: H38

Mitgliederversammlung der MM / Annual General Assembly of the MM Division

MM 47: Invited talk Leoni

Time: Thursday 9:30–10:00

Location: H38

Invited Talk

MM 47.1 Thu 9:30 H38

Nondestructive micro/nanostructure analysis using diffraction — ●MATTEO LEONI — DICAM, University of Trento, via mesiano 77 - 38123 Trento, Italy

In the past 100 years, powder diffraction evolved from being a solution to the problem of obtaining large single crystals, to a versatile tool for materials analysis. The diffraction pattern and in particular the breadth and shape of the profiles, bear information not just on the structure but also on the micro/nanostructure of a material, such as shape and size distribution of the domains and lattice defects. Technologically relevant systems show however peculiar features that can

hardly be interpreted as simple broadening effects, especially when modular features, 2D character or stacking defects are present: the local and global structures differ and a stochastic description of the specimens is needed. The recent advances in the field, well beyond the commonly misused Scherrer formula, allow all those cases to be quantitatively studied in a non-destructive way by refining physical structure and microstructure parameters directly on the data collected ex situ, in situ or operando. Virtual experiments and virtual models, as well as computational tools, can then be used to assess the capabilities of the analysis methods and to extract further information on defect structure, material characteristics and their evolution. An overview and some examples will be given.

MM 48: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science V - Biological and Electronic Materials

Time: Thursday 10:15–11:45

Location: H38

Topical Talk

MM 48.1 Thu 10:15 H38

In-situ TEM Switching of Non-volatile Memory Devices — ●SANG HO OH — POSTECH, 77 Cheongam-Ro. Pohang 37673, Republic of Korea

In this talk I will present two case studies illustrating how in-situ TEM is used to visualize the switching processes of non-volatile memory devices and to reveal the switching mechanisms. In the first example, the 180° polarization switching process of an epitaxial PbZr_{0.2}Ti_{0.8}O₃ (PZT) thin film capacitor is presented. The preferential, but asymmetric, nucleation and forward growth of switched c-domains were observed at the PZT/electrode interfaces, arising due to the built-in electric field induced at each interface. It was found that the preexisting a-domains split into fine a- and c-domains constituting a 90° stripe domain pattern during the 180° polarization switching process, revealing that these domains also actively participated in the out-of-plane polarization switching. In the second example, as a model resistive random access memory (ReRAM), I will show in-situ TEM observation of the multi-level switching of a TiN/Pr_{0.7}Ca_{0.3}MnO₃ (PCMO)-based ReRAM which utilizes the resistance change as the two materials goes through reversible redox reactions at the interface. Based on the direct observations of the microstructural evolution and correlated I-V characteristics, a resistive switching model for TiN/PCMO devices will be presented.

MM 48.2 Thu 10:45 H38

In situ studies of structural biological materials with X-ray microdiffraction — ●MARTIN MÜLLER — Helmholtz-Zentrum Geesthacht, Germany

The structural biological material silk combines high extensibility and high mechanical strength. The key to those unique mechanical properties lies in the hierarchically organised micro- and nanostructure with nanocrystals embedded in a softer, disordered matrix in the fashion of a composite material. Position-resolved in situ X-ray diffraction experiments play a central role in the development of new mechanical models, which also include the influence of humidity on the mechanical performance of silk. Based on our findings, native silk fibres were functionalised with chromophores in order to make them optically switchable; again, the mechanical switching effect is readily visible in X-ray microdiffraction experiments.

Further examples include the mechanical properties of wood and the attachment mechanism of adhesive spider hairs. Similarities with in situ experiments on engineering materials will be highlighted.

MM 48.3 Thu 11:15 H38

Microspectroscopic Insights into Electronic Switching — BENEDIKT RÖSNER¹, XIAOYAN DU¹, KE RAN², ERDMANN SPIECKER², MARAT M. KHUSNIYAROV³, and ●RAINER H. FINK¹ — ¹Physikalische Chemie II, FAU Erlangen-Nürnberg — ²CENEM, FAU Erlangen-

Nürnberg — ³Anorganische Chemie II, FAU Erlangen-Nürnberg

Controlling the electronic switching in metal-organic semiconductors is crucial for implementation of these materials into functional devices. We report on in-situ investigations of electronic switching with different microspectroscopic methods using electrons, X-rays and scanning probes. Bipolar resistivity switching in Ag-TCNQ nanocrystals is investigated using TEM, Raman-, and scanning X-ray transmission microspectroscopy. Reverse charge transfer within the charge transfer salt is demonstrated qualitatively and quantified [1]. In organic field-effect transistors, spatially resolved Raman spectroscopy proofs modifications of the polarizability tensor in the organic semiconductor upon operation, visualizing charge trapping [2]. Light-induced switching in our Fe(II) spin-crossover complex between a paramagnetic high-spin state and a diamagnetic low-spin state is proven using X-ray absorption and XPS. NEXAFS spectroscopy is thereby ideally suited to probe the d-orbital occupation and thus to quantify the fractions of the respective spin states [3]. This work is funded within the GRK 1896 (In-situ Microscopy with Electrons, X-rays and Scanning Probes). [1] B. Rösner et al., PCCP (2015), 17, p. 18278. [2] B. Rösner et al., Organic Electronics (2014), 15, p. 435. [3] B. Rösner et al., Angew. Chemie (2015) 54, p. 12976.

MM 48.4 Thu 11:30 H38

Natural silk made optically switchable — ●IGOR KRASNOV¹, NICOLAI R. KREKIEHN¹, CHRISTINA KRYWKA², ULRICH JUNG¹, AHNAF U. ZLOHU³, THOMAS STRUNSKUS³, MADY ELBAHRI^{2,3}, OLAF M. MAGNUSSEN¹, and MARTIN MÜLLER^{1,2} — ¹IEAP, Universität Kiel — ²Institute of Materials Research, HZG Geesthacht — ³Institut für Materialwissenschaft, Universität Kiel

An optically active bio-material is created by blending natural silk fibers with photoisomerizable chromophore molecules-azobenzenebromide (AzBr). The material converts the energy of unpolarized light directly into mechanical work with a well-defined direction of action. The feasibility of the idea to produce optically driven micro-sized actuators on the basis of bio-material (silk) is proven. [1] The switching behavior of the embedded AzBr molecules was studied in terms of UV/Vis spectroscopy. To test the opto-mechanical properties of the modified fibers and the structural changes they undergo upon optically induced switching, single fiber X-ray diffraction with a micron-sized synchrotron radiation beam was combined *in situ* with optical switching as well as with mechanical testing and monitoring. The crystalline regions of silk are not modified by the presence of the guest molecules, hence occupy only the amorphous part of the fibers. It is shown that chromophore molecules embedded into fibers can be reversibly switched between the *trans* and *cis* conformation by illumination with light of defined wavelengths.

[1] I. Krasnov et al., Applied Physics Letters, 106, 093702 (2015)

MM 49: Nanomaterials II: Synthesis

Time: Thursday 10:15–11:30

Location: H39

MM 49.1 Thu 10:15 H39

SOLIDIFICATION BEHAVIOUR OF INDIUM DROPLETS EMBEDDED IN AN ALUMINIUM MATRIX — ●MOSTAFA MOHAMED, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, Münster, Germany

A hypomonotectic alloy of Al-0.5-4 at% In has been manufactured by the melt-spinning technique. The microstructures of the embedded nanoparticles were investigated by transmission electron microscopy (TEM). As-melt spun alloy of Al-In consists of a homogeneous distribution of faceted particles formed during the monotectic solidification reaction.

The In nano-particles show a cube-cube orientation relationship with the surrounding Al-matrix. The kinetics of In particles solidification have been examined by heating and cooling experiments in a differential scanning calorimetry (DSC) over a range of heating and cooling rates. Analyses of the nucleation kinetics of In particles solidification

have been performed in the frame of the classical spherical cap model of heterogeneous nucleation.

MM 49.2 Thu 10:30 H39

Optical Nanoparticle Sorting Elucidates Synthesis of Plasmonic Nanotriangles — ●CHRISTOPH MAIER¹, MARIA A. HUERGO², MARCOS F. CASTEZ², CAROLINA VERICAT², ROBERTO C. SALVAREZZA², ALEXANDER S. URBAN¹, and JOCHEN FELDMANN¹ — ¹Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität, Amalienstraße 54, 80799 Munich, Germany — ²Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, Universidad Nacional de La Plata, Sucursal 4 Casilla de Correo 16, 1900 La Plata, Argentina

The synthesis of plasmonic nanoparticles by reducing gold salt by sodium sulfide leads to the formation of a strong near infrared (NIR) extinction peak [1], signifying strong potential for hyperthermic cancer

treatment. However, the nature of the underlying nanoparticles has been a matter of debate. Hybrid core-shell and gold nanoparticles with different shapes have been discussed. [2] We introduce wavelength selective optical printing in order to sort the synthesized nanoparticles according to their plasmon resonances. By arresting the synthesis at different times, we find that thin gold nanotriangles are responsible for the observed NIR resonance. We also discuss and explain the observed spectral shifts of the plasmon resonances as observed during synthesis. This novel method is applicable to other plasmonic nanoparticle syntheses. In the future, complex nanostructures can be built up on substrates by selectively printing nanoparticles of varying plasmonic resonances. [1] Zhou, H.S., et al., PRB 1994, 50, (16), 12052-12056 [2] Diao, J. J., et al., J. Chem. Phys 2006, 124, (11), 116103

MM 49.3 Thu 10:45 H39

Carbon Dots: A Unique Fluorescent Cocktail of Polycyclic Aromatic Hydrocarbons — ●FLORIAN EHRAT¹, MING FU¹, SANTANU BHATTACHARYYA¹, YU WANG², JACEK STOLARCZYK¹, ANDREY ROGACH², ALEXANDER URBAN¹, and JOCHEN FELDMANN¹ — ¹Photonics and Optoelectronics Group, Department of Physics, Ludwig-Maximilians-Universität (LMU), Munich, Germany — ²Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR

Carbon dots (CDs) have attracted rapidly growing interest due to their exceptional advantages such as high fluorescence quantum yield, chemical stability and biocompatibility. Recently the fluorescent CDs have been used for bioimaging, photocatalysis, photovoltaics, as light-emitting diodes, and for lasing. However, the intrinsic mechanism and origin of the fluorescence in CDs have not yet been completely understood.

We have recently developed a model system of polycyclic aromatic hydrocarbon (PAH) molecules embedded in a polymer matrix to reproduce the optical properties of CDs.[1] In particular, a large Stokes shift of more than 100 nm as well as excitation wavelength dependent emission properties could be achieved by fine-tuning of the concentration of only three different molecules. Therefore we conclude that these can be seen as the main emissive species within a CD. These results will help to enable specifically tailoring the optical characteristics of CDs.

[1] M. Fu, F. Ehrat, et al., Nano Lett. 2015, 15 (9), 6030-6035.

MM 49.4 Thu 11:00 H39

Anodic aluminum oxide: regularity evolution with time, temperature and underlying aluminum structure — ●STEFAN OSTENDORP, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, WWU Münster, 48149 Münster, Germany

Anodic aluminum oxide (AAO) has proven itself as a versatile tool

for nano-structuring purposes. Its ability to form a regularly arranged hexagonal pore array renders its utilization as a template or mask for the fabrication of zero- and one-dimensional nanostructures possible. Ever since pre-structuring and multistep anodizations have been introduced to yield regular through-hole structures, AAO has been used for the synthesis of different functional surface nano-structures. However, AAO growth and especially the regularity evolution under certain anodization conditions remained impossible to explain in a comprehensive way. Thus we focus in this work on quantitative investigations of AAO's regularity evolution with anodization time, temperature and with respect to the structure of the aluminum, the AAOs have been anodized from, to derive conditions for regular pore formation. Based on advanced anodization control as well as a graphical regularity analysis, AAOs fabricated under mild and hard anodization conditions have been studied and compared. It has been found, that the aluminum grain size and orientation has only a minor effect on the AAO's regularity. Moreover, there is actually no temperature dependence of the obtained regularity at all. Finally the regularity evolution with time revealed an electrolyte degeneration being responsible for sudden regularity loss, which might have been misinterpreted in previous works.

MM 49.5 Thu 11:15 H39

Computational study of fluorinated metal-organic frameworks applied to oil-water separation — ●JAMES MORAES DE ALMEIDA¹, CAETANO RODRIGUES MIRANDA², and NICOLA MARZARI¹ — ¹THEOS and NCCR MARVEL, EPFL, Lausanne, Switzerland — ²Nanopetro, Instituto de Física, USP, São Paulo, Brazil

Metal-organic frameworks (MOFs) have high surface areas and no lost space due to non-accessible volumes. Selective adsorption of fluids in MOFs is highly dependent on their surface properties, leading to a variety of applications. One example is oil-water separation, where MOFs can selectively adsorb oil molecules but not water - which is important to clean oil spills. MOFs with this property have been synthesized, typically with fluorinated surfaces (FMOFs - fluorinated MOFs). In this work, we perform first-principle simulations to study the interactions of FMOFs with several adsorbates: anthracene, naphthalene, phenol, heptane, benzene, benzoic-acid, toluene, methane and water. The calculated binding energies show that, with an exception of the methane, all hydrocarbons have stronger binding to the FMOFs. In addition, we analyzed the location of the HOMO and LUMO orbitals. While the LUMO is never found on the adsorbate, the HOMO (or at least the HOMO-1) can sit on the molecules for several cases - anthracene, benzene, naphthalene, benzoic-acid and toluene - making these all available for chemical reactions. Last, while hydrocarbons interact strongly with FMOFs, water still has a favorable adsorption energy, but will be displaced by all the hydrocarbons considered, but methane.

MM 50: Methods in Computational Materials Modelling II: Microstructure evolution

Time: Thursday 10:15–11:45

Location: H53

MM 50.1 Thu 10:15 H53

Atomistic insight into the structure and shape of growing nuclei during solidification in Ni — ●GRISELL DIAZ LEINES, RALF DRAUTZ, and JUTTA RO GAL — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

A crucial stage during solid-liquid phase transformations is the initial nucleation of a stable phase within a metastable medium. Molecular dynamics simulations provide an atomistic picture of solidification, but the modelling of the initial nucleation is hampered by the extended timescale of the process. In this work we employ an advanced computational method, transition path sampling (TPS), to enable the investigation of nucleation in elemental nickel on the atomistic level. We initially focus on homogeneous nucleation. Here, a comparison of the temperature dependence of the free energy barriers to the predictions of classical nucleation theory is discussed. As a second step, we extend our study by including small Ni-clusters as seeds during heterogeneous nucleation. The analysis of the transition path ensemble (TPE) obtained from our simulations indicates the presence of fcc and hcp crystalline structures and nonspherical shapes of the clusters. Furthermore, critical nuclei sizes, free energy barriers and rates, as well as optimal candidates for reaction coordinates based on local structural

parameters are identified in the TPE. These results provide fundamental understanding of the nucleation mechanisms and can help to validate and improve existing thermodynamic models describing nucleation in metals.

MM 50.2 Thu 10:30 H53

Derivation of TTT diagrams with kinetic Monte-Carlo simulations — ●ANKIT GUPTA, BISWANATH DUTTA, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Al-based light-weight alloys are promising for structural applications. A critical strengthening mechanism in these alloys is precipitate formation and thus the inherent evolution of the precipitates over time plays a key role in governing the mechanical behaviour of these alloys. Therefore, in order to fine tune the mechanical properties, an in-depth understanding of the precipitation kinetics is crucial. In this work, we study the precipitation kinetics in a model Al-Sc system employing kinetic Monte-Carlo (kMC) simulations. A linear bond-cutting model has been used to describe the underlying energetics. The kinetics has been analysed in terms of size distribution of the precipitates and their temporal evolution. The final results have been plotted as time-temperature-transformation (TTT) diagrams. The critical factors controlling the key features of the fully atomistically derived

TTT diagrams such as asymptotic and nose temperature are discussed. Since the key observations are independent of the specific material system, they can be applied to tailor the precipitation kinetics in many applications.

MM 50.3 Thu 10:45 H53

On the Propagation of two en passant cracks upon mutual interaction: A phase field study — ●MICHAEL FLECK, MARKUS THÄTER, MARTIN LAUTENSCHLÄGER, and HEIKE EMMERICH — Materials and Process Simulation, University of Bayreuth, Germany

A phase field model for the simulation of crack propagation in brittle materials is applied to the problem of two mutually interacting "en passant" cracks. Thereby, crack growth is described as a first order phase transformation process, where the solid parent phase transforms into an infinitely weak "broken" phase, driven by elastic energy dissipation. We discuss the problem of "en passant" cracks in a two dimensional plain strain geometry, subjected to a constant uniaxial pulling velocity of mode I type. Our model reproduces a number of basic features that are also observed in corresponding experimental setups. Initially, when the two cracks propagate independently, they approach each other along straight paths. Then, during the early stage of the mutual interaction and for certain geometrical circumstances the principle of local symmetry may even force the cracks to turn slightly away from each other. When the line connecting the two crack tips aligns with the pulling direction, the two cracks curve towards each other upon mutual tip-tip interaction until each crack tip reaches the other's crack tail, finally releasing a lenticular fragment. Here, we investigate the crack propagation dynamics as well as the chosen crack paths as a function of all relevant physical dependences, with the aim to elucidate the governing mechanisms that allow to classify the observed kinetics.

MM 50.4 Thu 11:00 H53

Laser Ablation of Alloys and Layered Materials — ●JOHANNES ROTH¹, DENNIS RAPP², ALEXANDER KISELEV¹, and HANS-RAINER TREBIN¹ — ¹FMQ, Universität Stuttgart — ²IWMF, Universität Stuttgart

We have studied laser ablation of Al-Ni alloys and layers using MD simulations combined with a two-temperature model (TTM) to describe the influence of the electrons. First the simulation program had

to be adapted to alloys and the parameters for the electronic contribution had to be determined. After tests with pure Al and Ni melting depths and ablation thresholds for AlNi, AlNi₃ and Al₃Ni have been determined. For AlNi₃ we observe a change in ablation mechanism at high fluences and for the orthorhombic Al₃Ni a phase transition to a cubic L1₂ phase. Unfortunately there are nearly no experimental data available to compare with.

Al layers on Ni substrates have also been studied. A thin layer of Al melts first, the Ni substrate follows, then the Al is ablated completely. A thicker Al layer absorbs a lot of laser energy and delays the melting of the Ni substrate to considerably higher fluences. At fluences low above the ablation threshold the thick Al layer is ablated as a whole as before, but at higher fluence the ablation depth is reduced due to vaporization of Al which cools the sample. The diffusion assisted formation of AlNi alloys has been observed in the thin layer case for fluences close to the ablation threshold. The structure of the compounds is fcc as in AlNi, but the composition varies from pure molten Al to solid Ni.

MM 50.5 Thu 11:15 H53

Impurity diffusion in bcc-iron from first-principles — ●CASPER VERSTEYLEN¹ and MARCEL SLUITER² — ¹Mekelweg 2, 2628 CD Delft, the Netherlands — ²Mekelweg 15, 2629 JB Delft, the Netherlands

Since detailed knowledge of impurity diffusivities is vital in the design of new steel compositions and microstructures, substitutional diffusion in bcc-iron has been studied comprehensively. Calculating diffusivities at temperatures relevant for realistic applications is difficult for several reasons; accurate excess entropies must be determined for vacancy formation and element specific vacancy binding while accounting for magnetic disordering. Sophisticated techniques have been developed to evaluate the influence of magnetism on total energies, but to do so for a large number of impurity elements in iron is expensive. Therefore a method was developed that links first principles results to the semi-empirical Girifalco model. A general method to evaluate the influence of magnetic disordering on impurity diffusivities has been applied to 28 impurity elements in bcc-iron and to iron self-diffusion.

15 min. coffee break

MM 51: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV

Time: Thursday 10:30–13:15

Location: H24

Topical Talk

MM 51.1 Thu 10:30 H24

Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — ●IVO SOUZA — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies ("Weyl points") in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a "gyrotropic magnetic effect" (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk

MM 51.2 Thu 11:00 H24

Dirac Fermions in Antiferromagnetic Semimetal — ●PEIZHE TANG, QUAN ZHOU, GANG XU, and SHOU-CHENG ZHANG — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems

have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

MM 51.3 Thu 11:30 H24

Spin Hall effect in non-collinear antiferromagnets Mn₃X (X=Sn, Ge, Ga) — ●YANG ZHANG^{1,3}, YAN SUN¹, CLAUDIA FELSER¹, and BINGHAI YAN^{1,2} — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany, ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ³Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in non-collinear antiferromagnetic (AFM) compounds Mn₃X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [~ 1000 ($^*/e$)(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for

the room-temperature spintronic applications.

MM 51.4 Thu 11:45 H24

Electronic reconstruction and anomalous Hall conductivity in 3d-oxide honeycomb lattices within the corundum structure — ●SANTU BAIDYA and ROSSITZA PENTCHEVA — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of 3d transition metal oxide honeycomb layers confined in the corundum structure (α -Al₂O₃) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. (M₂O₃)/(Al₂O₃)₅, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound M₂O₃, strong deviations from the bulk behavior are observed in the case of Ti₂O₃ and Mn₂O₃ bilayers. Our results indicate a formation of a quasi two-dimensional electron gas with a vertical confinement of ~ 5 Å for Ti₂O₃ and ~ 8.5 Å for Mn₂O₃. As a function of lateral strain (Ti₂O₃)/(Al₂O₃)₅ undergoes a metal-to-insulator transition associated with a switching of orbital polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in (M₂O₃)/(Al₂O₃)₅ (M=Ti, Mn).

MM 51.5 Thu 12:00 H24

Anomalous hall effect in triangular antiferromagnetic ordered structure — ●HAO YANG¹, SUN YAN², FELSER CLAUDIA², PARKIN STUART¹, and BINGHAI YAN² — ¹Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — ²Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn₃X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

MM 51.6 Thu 12:15 H24

Anomalous Hall conductivity and orbital magnetization as local quantities — ●ANTIMO MARRAZZO¹ and RAFFAELE RESTA² — ¹THEOS, EPF Lausanne, Switzerland — ²Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist's viewpoint—closely related: both have an expression as \mathbf{k} -space integrals of the appropriate geometrical quantity. The \mathbf{k} space is an artificial construct: all bulk properties are embedded in the ground state density matrix in \mathbf{r} space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in \mathbf{r} space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the “nearsightedness” of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic \mathbf{B} field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

MM 51.7 Thu 12:30 H24

Laser induced DC photocurrents in a Topological Insulator thin film — ●THOMAS SCHUMANN¹, NINA MEYER¹, GREGOR MUSSLER⁴, EVA SCHMORANZEROVÁ², DAGMAR BUTKOVICOVA², HELENA REICHLIOVÁ³, LUKAS BRAUN⁵, CHRISTIAN FRANZ⁶, MICHAEL CZERNER⁶, PERTR NĚMEC², DETLEV GRÜTZMACHER⁴, TOBIAS KAMPFRATH⁵, CHRISTIAN HEILIGER⁶, and MARKUS MÜNZENBERG¹ — ¹IfP, EMA University Greifswald, Germany — ²MFF, Charles University, Prague, Czech Republic — ³FZU, Prague, Czech Republic — ⁴PGI-9, Jülich, Germany — ⁵FHI Berlin, Germany — ⁶University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent. We report our recent results on laser induced photocurrents in a ternary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev, W.Prettl, J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver, D.Hsieh, H.Steinberg, P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

MM 51.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — ●CHRISTIAN TUTSCHKU¹, ROLF W. REINTHALER¹, CHAO LEI², ALLAN H. MACDONALD², and EWELINA M. HANKIEWICZ¹ — ¹Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — ²Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

[1] A. Y. Kitaev, Physics-Uspekhi 44, 131 (2001)

[2] D. A. Ivanov, PRL 86, 268 (2001)

[3] J. Alicea et al., Nature Physics 7, 412 (2011)

MM 51.9 Thu 13:00 H24

Unpaired Majorana modes in Josephson junctions arrays with gapless bulk excitations — ●MANUEL PINO GARCIA — Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 Frelinghuysen rd, Piscataway, 08854 New Jersey, USA

The search for Majorana bound states in solid-state physics has been limited to materials which display a gap in their bulk spectrum. We will show that such unpaired states appear in certain quasi-one-dimensional Josephson junctions arrays with gapless bulk excitations. The bulk modes mediate a coupling between Majorana bound states via the Ruderman-Kittel-Yosida-Kasuya mechanism. As a consequence, the lowest energy doublet acquires a finite energy difference. For realistic set of parameters this energy splitting remains much smaller than the energy of the bulk eigenstates even for short chains of length $L \sim 10$. In this talk, we first explain the JJA system and how to model it with an Ising-like Hamiltonian. Then, a qualitative argument is employed to obtain the low-energy effective theory using unpaired Majorana modes. We will show numerical results which confirm the validity of this effective theory and discuss problems that may arise in the experimental realization of our proposal.

MM 52: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science VI - Structural transitions

Time: Thursday 11:45–13:15

Location: H38

15 min. coffee break

MM 52.1 Thu 12:00 H38

Grain growth of nc-Pd during heating using ACOM-STEM — ●KK NEELISETTY^{1,4}, A KOBLE^{1,4}, VSK CHAKRAVADHANULA^{1,3,4}, T SCHERER^{1,2}, H HAHN^{1,3,4}, and C KÜBEL^{1,2,3} — ¹INT, Karlsruhe Institute of Technology (KIT), Germany — ²KNMF, KIT, Germany — ³HIU, KIT, Germany — ⁴TU Darmstadt, Germany

Understanding grain growth in nanocrystalline (nc) metals and how it can be controlled and tuned is a major objective for applications and provides new fundamental insights. In-situ heating experiments in TEM using Automated Crystal Orientation Mapping (ACOM) is a powerful approach to reveal the microstructure and orientation of grains in nanoscale and follow its structural evolution. In this study, sputtered ncPd thin-films about 50 nm thick were used to evaluate the grain growth in 2D. Mapping grain orientation in an area initially containing more than thousand grains with a resolution of 1.5 nm allowed for a statistically meaningful analysis of grain orientation, presence of twins, grain rotation and grain boundary migration over time at elevated temperature. Evaluation of maps was performed using MATLAB using Mtex tool-box, providing information about the local misorientations between grains, CSL boundary, twin density and grain size distribution, texture, and number of neighbors of selected growing grains. Global analysis of grains growing is in good agreement with the structural changes observed in bulk samples. Local analysis shows that grain boundary curvature and grain boundary angle are not sufficient criteria to explain grain growth in nc-metals, but triple- and quadruple line networks appear to stabilize nanograins locally.

MM 52.2 Thu 12:15 H38

Solid-state Dewetting of Metallic Thin Films Studied by Complementary in situ Transmission Electron Microscopy Techniques — ●FLORIAN NIEKIEL, SIMON M. KRASCHEWSKI, PETER SCHWEIZER, BENJAMIN BUTZ, and ERDMANN SPIECKER — Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nürnberg, Erlangen, Germany

The transition of a thin film into an energetically favorable set of particles at temperatures below the melting temperature of the bulk material is denominated as solid-state dewetting. This phenomenon is on the one hand an undesirable degradation and failure mechanism in thin film applications. On the other hand it can deliberately be exploited to generate nanoparticle arrays with controlled shape, ordering and composition.

In this work we use complementary in situ transmission electron microscopy (TEM) techniques with a chip-based heating system to study the underlying physics during solid-state dewetting. The techniques employed range from electron diffraction over scanning transmission electron microscopy (STEM) to high-resolution TEM. The combination of statistical information with microscopical information down to the atomic scale provides insights into the kinetics, texture evolution and mechanisms involved.

MM 52.3 Thu 12:30 H38

Suppression of phase transformations in Nb-H thin films — ●VLADIMIR BURLAKA, STEFAN WAGNER, and ASTRID PUNDT — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Mechanical stress in the GPa-range is known to arise during hydrogen absorption in metal films adhered to rigid substrates.[1] It can be released by plastic deformation. For thin films, stress release is much less efficient than for thicker films: It can be even suppressed, and very thin films can stay in a highly stressed state.[2] This influences the thermodynamic and kinetics properties of the system, and may suppress phase transformations.[3] In this presentation, we use Nb-H films as a model system to study the presence of phase transformations depending on the film thickness ($d < 110$ nm). Phase transformations

can be monitored by studying surface corrugations with the scanning tunneling microscope (STM).[4] As soon as hydride precipitates form inside the metal film, a local height change will be detected in the film surface topography. We have demonstrated that this method is more sensitive than conventional XRD.[5] STM allows for finding a Nb-film thickness, below which no sign of a phase transformation can be found at 300K. Complementary methods support this experimental result. This research is kindly supported by the DFG via the projects PU131/12-1 and PU131/9-2. [1] A. Pundt et al. Annu. Rev. Mater. Res. 36 (2006) 555. [2] M. Hamm et al., APL 106 (2015) 243108. [3] S. Wagner et al., Int.J.Hydr.En., in print. [4] K. Nörthemann et. al., PRB 78 (2008) 014105. [5] V. Burlaka et al., JALCOM 645 (2015) 388.

MM 52.4 Thu 12:45 H38

Influence of patterned stress states on hydrogen loading in Vanadium thin films studied by electrochemical hydrogenography — ●ANSHU TYAGI, FLORIAN DÖRING, HANS-ULRICH KREBS, and ASTRID PUNDT — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

It has been shown that the mechanical stress state of a metal film sensitively affects the chemical potential of hydrogen in the metal.[1] The stress state of a film can be changed by the adhesion of the metal film to the substrate and can be modulate by patterning the adhesion conditions. [2] Stress sensitive Vanadium thin films act as model systems in this work. These films are sputter deposited onto transparent glass substrates. Patterning is performed using Palladium and Polycarbonate layers. The hydrogen uptake in these films is studied using Hydrogenography which monitors the film transparency and reflectivity.[3] We apply this method using electrochemical loading in a light-microscope. This electrochemical Hydrogenography allows to optically probe for the local hydrogen concentration.

Comparative studies on different adhesion conditions are done by in-situ EMF measurements. This provides the related chemical potentials including information about the phase boundaries. The transmission and reflection spectra are discussed with respect to these data.

References [1] S.Wagner, A. Pundt, APL 92 (2008) 051914. [2] A. Pundt, E. Nikitin, R. Kirchheim, P. Pekarski, Acta Mater. 52 (2004) 1579. [3] R. Gremaud, M. Slaman, H.Schreuders, B.Dam, and R.Griessen, APL 91 (2007) 231916.

MM 52.5 Thu 13:00 H38

Transmission electron microscopy image and energy-dispersive X-ray map simulations of Ga-covered Pb nanoparticles embedded in an Al matrix. — ●MARTIN PETERLECHNER and GERHARD WILDE — Institut für Materialphysik, WWU Münster, Münster, Deutschland

Nanoparticles are in focus of research since decades due to their size effects. Embedded nanoparticles in a matrix show additional effects caused by their interface structure. In the present study, the simulation of transmission electron microscopy (TEM) images is focused. High-resolution TEM (HRTEM) contrast, Scanning-TEM (STEM) contrast and energy-dispersive X-ray (EDX) maps are elucidated. A simple atomistic model of an Al matrix with Ga-covered embedded Pb nanoparticles was chosen to study moiré contributions and thickness effects for contrast formation. HRTEM images of the as-generated structures were simulated using the multislice algorithm by Kirkland, and STEM/EDX micrographs were simulated using muSTEM by D'Alfonso, Findlay and Allen. The spacing of the moiré pattern can be used to determine the difference of the involved lattice planes with a high accuracy, however, measurements of absolute atomic positions are not always possible since atoms can become 'invisible' at local regions of the moiré pattern. Moreover, apparent interface roughening can occur by moiré effects. The EDX signal of the Ga atoms is blurred with increasing thickness. Therefore, image simulation is inevitable to interpret atomic positions and chemistry at interfaces, in particular when a nanoparticle is embedded and not of constant thickness.

MM 53: Microstructure and Phase Transformations II

Time: Thursday 11:45–13:00

Location: H39

MM 53.1 Thu 11:45 H39

Phase Transformation in Alloyed Nanowires — ●MANUEL ROUSSEL, MARTIN SCHELLENBERGER, TIM LEHMANN, and GUIDO SCHMITZ — Institute for Materials Science, Stuttgart, Germany

Since the discovery of giant magnetoresistance, for which Albert Fert and Peter Grünberg have been awarded the 2007 Nobel Prize, thin magnetic films have attracted much interest. More particularly, multi-layered nanowires consisting of magnetic and nonmagnetic layers (FeNi/Cu, Ni/Cu, Fe/Cr, Co/Cu...) have been proven to exhibit outstanding properties which have straightforward applications: MRAM (magnetic random access memories), nano-sensors, data storage... Most of the time, the bottle neck for the usage of such nanostructures is that their synthesis is not reliable, especially when it comes to producing very small wires, in the range of a few tens of nanometers diameter. We are exploring alternative synthesis routes in order to find a new self-ordering way of producing multilayered or core-shell nanowires which would be only based on diffusion processes and phase separation. Simply put, we would like to create a plain alloyed nanowire and provoke the formation of layers just by a well-designed heat treatment. We will first present our approach to grow alloyed metallic nanowires of various compositions. In order to do so, we adopted a process based on electro-deposition in porous membranes. Later on we will focus on the influence of the nanowire geometry on phase transformation during annealing.

MM 53.2 Thu 12:00 H39

Core-shell structure of precipitates in the Al-Sc-Zr system — ●YULIA BURANOVA¹, ANKIT GUPTA², VLADISLAV KULITCKII³, TILMANN HICKEL², SERGIY V. DIVINSKI¹, and GERHARD WILDE¹ — ¹Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — ²Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf 40237, Germany — ³Laboratory of Mechanical Properties of Nanoscale Materials and Superalloys, Belgorod State University, Pobeda 85, Belgorod 308015, Russia

Aluminum alloys containing scandium show excellent mechanical properties due to the presence of Al₃Sc precipitates, which control the dislocation and grain boundary motion during the recrystallization processes. An addition of Zr can further improve the properties due to the formation of Al₃(Sc,Zr) dispersoids, which are more stable at elevated temperatures. In this work we investigate a commercial aluminum alloy AA5024, containing Sc, Zr, Ti and Mg additions. The particles size, chemistry and distribution were investigated by analytical transmission electron microscopy and geometric phase analysis was applied to map local strains. It is found that the Al(Sc,Zr,Ti)-precipitates reveal complex core-shell structures which are strongly affected by mechanical deformation and heat treatment. The experimental findings are compared with predictions based on DFT calculations, which indicate the existence of a critical size for the appearance of ternary Al₃(Sc,Zr) shells. The financial support of DFG within SPP 1713 is gratefully acknowledged.

MM 53.3 Thu 12:15 H39

Mechanical behaviour and deformation mechanisms of a Zn-Al-Cu-Mg alloy — ●ZHICHENG WU, STEFANIE SANDLÖBES, GÜNTER GOTTSTEIN, and SANDRA KORTE-KERZEL — Institut für Metallkunde und Metallphysik, RWTH Aachen, D-52056 Aachen, Germany

The microstructure, mechanical properties and deformation behaviour of a gravity-cast alloy ZnAl₄Cu₁Mg_{0.3} (wt.%) was studied at different temperatures and strain rates using ex-situ and in-situ tensile tests in conjunction with scanning electron microscopy, electron backscatter

diffraction, transmission electron microscopy and atom probe tomography. The alloy revealed two distinct deformation regimes, i.e. work hardening and brittle fracture at room temperature and/or elevated strain rates, and work softening and ductile fracture at elevated temperatures and/or low strain rates. Further, we identified precipitates of a non-equilibrium Zn_xAl_{1-x} (x≥0.7) transition phase or Guinier-Preston zone which partly dissolved during deformation at elevated temperatures. The partial dissolution of these precipitates is assumed to partially account for the observed increase in ductility at elevated temperatures, but might also contribute to the long-term softening of Zn-Al alloys that currently poses one of the major drawbacks to their application.

MM 53.4 Thu 12:30 H39

Zener ordering of interstitials in a bcc host lattice: Interplay between short- and long-range interactions — ●XIE ZHANG¹, TILMANN HICKEL¹, JUTTA RO GAL², and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — ²Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44780 Bochum, Germany

The octahedral interstitial sites in a bcc lattice can be categorized into three sublattices that can be occupied with interstitials and that are characterized by the corresponding tetragonal deformation variants ([100], [010] and [001]). Even in an external stress-free system, the interstitials energetically prefer to occupy only one of the three sublattices below a critical temperature. This preference is triggered by the interactions between the interstitials and termed Zener ordering. Although it was proposed by Zener more than half a century ago, direct proofs from atomistic simulations have been, however, rarely reported so far, which even resulted in a debate on the validity of such ordering recently. Hence, in this work, we employ atomistic simulations to directly investigate the interplay between long-range strain induced and short-range chemical interactions. It is found that a homogenized distribution of interstitials within one octahedral sublattice is crucial, and ensures that the short- and long-range interactions are minimized simultaneously. These insights help to understand self-induced collective ordering of interstitials within a bcc host lattice which is a key mechanism to harden steels.

MM 53.5 Thu 12:45 H39

Multi-scale modeling of phase transitions around dislocations — ●GERARD PAUL LEYSON, BLAZEJ GRABOWSKI, and JÖRG NEUGEBAUER — Max Planck Institute for Iron Research, Max-Planck-Straße 1, 40237 Düsseldorf

Classic nucleation theory does not take into account local stress gradients present in the material. In particular, the stress field around a dislocation is large and can provide a strong driving force for phase transition and stabilize phases that would otherwise be unstable in the unstressed bulk material. To describe the impact of dislocation strain on nucleation we have developed a multi-scale framework. First, classic nucleation theory is generalized to include the effects of external stress gradients. As input the dislocation stress field is determined using a semi-empirical embedded atom (EAM) method. Second, the change in formation energy due to the phase transformation is calculated using ab-initio calculations. Using this approach we identify conditions that lead to a quasi-one-dimensional defect that is stable against coarsening. The mechanism identified here is general and applies e.g. to the recently found linear complexions in Fe-Mn alloys [1] or the formation of nano-hydrides at dislocations [2].

[1] Kuzima M, Herbig M, Ponge D, Sandlöbes S and Raabe D. Science 2015; 349: 1080-1083. [2] Leyson GP, Grabowski B and Neugebauer J. Acta Materialia 2015; 89:50-59

MM 54: Biomaterials and Biopolymers II (Joint CPP/BP/MM)

Time: Thursday 11:45–13:00

Location: H52

MM 54.1 Thu 11:45 H52

Stimuli responsiveness of electron irradiated gelatin — •STEFANIE RIEDEL^{1,2}, EMILIA I. WISOTZKI^{1,2}, KATHARINA APEL¹, WOLFGANG KNOLLE¹, and STEFAN G. MAYR^{1,2} — ¹Leibniz-Institut für Oberflächenmodifizierung, Leipzig — ²Fakultät für Physik und Geowissenschaften, Universität Leipzig

Stimuli responsive materials have attracted considerable interest during the past years due to their potential use in sensor and actuator applications. They are designed to transform small external stimuli e.g. temperature and humidity changes into a significant response.

While a large number of alloys or synthetic polymers are well-established at this point, we explore the potential of the biomaterial gelatin to respond to humidity changes. We demonstrate how irradiation with high-energetic electrons allows fine-tuning of the response. In addition, this treatment enhances thermal stability providing high attractiveness for biomedical applications.

MM 54.2 Thu 12:00 H52

Langzeitverhalten von Seide und "Selbstheilung" — •JAN ROSIGKEIT¹, IGOR KRASNOV¹ und MARTIN MÜLLER^{1,2} — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel — ²Institut für Werkstofforschung, Helmholtz-Zentrum Geesthacht

Durch Streckexperimente haben wir mechanische Eigenschaften des biologischen Nanokomposits Seide unter Verwendung eines Modells aus der linearen viskoelastischen Theorie [1] über lange Zeiten bestimmt. Wir stellen fest, dass sich die mechanischen Eigenschaften der Seide auf langen Zeiten "fraktional" viskoelastisch ("Memory"-Effekt) beschreiben lassen.

Seidenfasern können sich in zwei Zuständen befinden. Einer dieser Zustände ist ein stabiler Zustand der nicht vorgestreckten Faser. Der andere Zustand wird durch äußere Krafteinwirkung hervorgerufen, wodurch eine vorgestreckte Faser entsteht. Wir haben experimentell gezeigt, dass der Übergang vom vorgestreckten zum Anfangszustand in einer nassen Umgebung innerhalb von 24 Stunden stattfindet. Der vorgestreckte Zustand ist daher ein metastabiler Zustand. [2]

[1] W. Glöckle und T. Nonnenmacher, *Macromol.*, **24**:6426-6434 (1991).

[2] J. Rosigkeit, Bachelorarbeit, Christian-Albrechts-Universität Kiel (2014).

MM 54.3 Thu 12:15 H52

Fractional dynamics in silk — •IGOR KRASNOV¹, TILO SEYDEL³, and MARTIN MÜLLER² — ¹IEAP, Universität Kiel, Germany — ²Institute of Materials Research, HZG, Germany — ³ILL, Grenoble, France

Structural relaxations in humid silk fibers exposed to tensile stress have been observed to take place on a very wide range of time scales from a few milliseconds to several hours. The time-dependence of the measured tensile force following a quasi-instantaneously applied external strain on the fibers can be understood in terms of a fractional vis-

coelastic relaxation function introducing memory effects by which the mechanical state of a fiber depends on its tensile history. [1] An analog fractional relaxation also gives rise to the subdiffusion observed on picosecond time scales, which governs the mobility of the amorphous polymer chains and adsorbed water on the molecular level. The reduction of the subdiffusive memory effect in stretched fibers compared to native fibers is consistent with the higher order of the polymers in the stretched state.

[1] I. Krasnov, T. Seydel, and M. Müller, *Phys. Rev. E* **91**, 042716 (2015)

MM 54.4 Thu 12:30 H52

Mechanical properties of branched actin filaments — •MOHAMMADHOSEIN RAZBIN¹, MARTIN FALCKE^{3,4}, PANAYOTIS BENETATOS⁵, and ANNETTE ZIPPELIUS^{1,2} — ¹Georg August University — ²Max Planck Institute for Dynamics and Selforganization — ³Humboldt University — ⁴Max Delbrueck Center for Molecular Medicine — ⁵Kyungpook National University

Motile cells on a 2dimensional substrate generate motion by flat membrane protrusion called lamellipodia. Within lamellipodia, actin filaments are generated by branching off existing ones, giving rise to branched network structures. We investigate the force-extension relation of branched actin filaments, grafted on an elastic substrate at one end and pushing with the free ends against a flat and stiff wall. We compute the thermal fluctuation of the endpoints and the resulting entropic forces on a membrane, restricting the fluctuations of the endpoints. The entropic forces are shown to depend sensitively not only on the persistence length but also on the geometry of the structure. It depends on branch point position and filament orientation, being most pronounced for intermediate tilt angles and intermediate branch point positions. We describe filament networks without cross-linkers to focus on the effect of branching. We compare properties of branched and unbranched networks. The ratio of the network average of the force per branched filament to the average force per unbranched filament exhibits compression dependence and may go up to about 4.5 in networks with a narrow orientation distribution. With orientation distributions measured in lamellipodia, it is about 2.

MM 54.5 Thu 12:45 H52

Tension, Balance and Flex: Auxetic periodic tensegrities — •MYFANWY EVANS — TU Berlin, Berlin, Germany

We present here a class of triply-periodic tensegrity structures that have a negative Poisson's ratio: they are auxetic. These theoretical materials are derived from periodic rod packings or more general periodic filament packings with a dilatant property. We show that these chiral tensegrity structures are periodically rigid but affinely flexible. The affine flex leads to isotropic expansion or contraction. A parallel can be drawn between these tensegrity structures and woven materials with elastic filaments, which also display an auxetic behaviour. Such materials are an exciting target for functional materials and biomaterials, from metal-organic frameworks to woven polymeric or filamentous structures.

MM 55: Methods in Computational Materials Modelling III: Machine learning and statistics

Time: Thursday 11:45–13:00

Location: H53

MM 55.1 Thu 11:45 H53

Gaussian approximation potentials: the case of α -iron — •DANIELE DRAGONI¹, TOM DAFF², GÁBOR CSÁNYI², and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials (THEOS), and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École polytechnique fédérale de Lausanne, 1015 Lausanne, Switzerland — ²Engineering Laboratory, University of Cambridge, Trumpington Street, Cambridge, CB2 1PZ, United Kingdom

Interatomic potentials are typically based on functional forms driven by physical intuition and fitted to experimental or computational data. The moderate flexibility of these functional forms limits their ability to be systematically improved by increasing the fitting datasets, although ensuring a modicum degree of transferability. Recently, a novel

trend has emerged where potential-energy surfaces are represented by neural networks fitted on large numbers of first-principles calculations, thus maximizing flexibility but requiring extensive datasets to ensure transferability. Gaussian Approximation Potentials in particular are a novel class of potentials based on non-linear, non-parametric Gaussian-process regression. We apply this approach to the case of α -iron, training a GAP model from energies, stresses and forces taken from first-principles molecular dynamics simulations of pristine and defected bulk systems, and of surfaces with different crystallographic orientations, covering roughly 10^9 local atomic environments. Finally, we verify this GAP model by comparing its predicted structural, vibrational, and thermodynamic properties against those derived from first-principles.

MM 55.2 Thu 12:00 H53

Local Pattern Discovery for Uncovering Physically Interpretable Characterizations of Material Configurations — ●MARIO BOLEY, BRYAN R. GOLDSMITH, LUCA M. GHIRINGHELLI, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin.

Currently, machine learning applications to data from atomistic material simulations mostly focus on the inference of a global prediction model for some quantities of interest, such as (relative) energies. However, due to their global prediction-based objective, these models are usually not well suited for the discovery of physically interpretable characterizations of *local* groups of subsets of material, in particular when aiming at partitioning the configurational space of a system at finite temperature.

In contrast to predictive global modelling, local pattern discovery techniques directly aim to uncover specific local properties of the data. Moreover, they describe these properties through models that are built from discrete symbols corresponding to meaningful notions of the discovery domain. Therefore, they constitute an important complementary part of the data mining toolbox for the automatic analysis of materials-science data repositories. As an exemplary application of local pattern discovery for materials science, we consider the automatic discovery of configurational basins of gold clusters and their characterization in terms of interpretable features such as their coordination histogram and their moments of inertia, or (non-linear) functions of those features.

MM 55.3 Thu 12:15 H53

Automated Convergence Checks with the Python Based Library PyIron — ●JAN JANSSEN, TILMANN HICKEL, and JOERG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Over the last years methodological and computational progress in atomistic simulations has substantially improved the predictive power in materials design. To guarantee the desired numerical precision, simulation tools that run the necessary complex simulation protocols and convergence checks automatically are critical but scarce. Based on our recently developed PyIron library which provides an efficient framework to implement such protocols we have developed an automatized tool for fitting the Birch-Murnaghan equation of states with prescribed accuracy targets. The tool includes an approach to handle the intrinsic energy fluctuation in DFT simulations. By making a Monte-Carlo based sensitivity analysis that includes the intrinsic model errors as well as the energy fluctuations we determine the numerically most efficient volume range for the approximation. The achievable accuracy as well as the performance gains of such an approach will be discussed.

MM 55.4 Thu 12:30 H53

Examination of electrolyte diffusion in dye-sensitized solar cells using virtual random walk — ●TOMASZ BLACHOWICZ¹, ANDREA EHRMANN², HAFED ZGHIDI³, and MAKSYM WALCZAK³ — ¹Silesian University of Technology, Institute of Physics, Gliwice, Poland — ²Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld (Germany) — ³Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice (Poland)

Statistical analysis of optically captured microphotographs revealing different physical phenomena is an important research tool, supporting other standard experimental and theoretical research efforts. The statistical analysis relies on performing a virtual random walk on positions where the matter exists. Thus, this is especially suited for spatial and structural analysis of different materials.

The method enables recognition, in a quantitative way, and characterization of difference spatial elements, their sizes and frequencies of occurrence. A parameter describing these properties is so called Hurst exponent.

In the current work, results from analysis of different scenarios from liquid/solid state interaction at interfaces, e.g. dyestuff on TiO₂ layers on glass or textile, are examined. Image sequences obtained enable identification of uniformity levels for the liquid phase spread on a solid substrate.

MM 55.5 Thu 12:45 H53

Quantitative analysis of the interface layers in textile-3D print composites by image processing — ●ANDREA EHRMANN¹, TOMASZ BLACHOWICZ², HAFED ZGHIDI³, MAKSYM WALCZAK³, and NILS GRIMMELSMANN¹ — ¹Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld, Germany — ²Silesian University of Technology, Institute of Physics, Gliwice, Poland — ³Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice (Poland)

Computational materials modeling is nowadays standard research technique as a counterpart to classical experimental and theoretical activity.

In this work we identify different solid-state phases derived from analysis of grey-scaled two-dimensional images captured optically. An original image was split into virtual sub-layers falling into different ranges at the grey-level level. Numerical analysis performed at the sub-images was carried out using a random walk approach. The method enables quantitative diagnosis of different material components and differentiation between samples prepared at different physical conditions.

We will depict results of cross section micrographs taken from FDM printing with different thermoplastics on textile substrates, allowing for giving a quantitative description of the interface layer structure.

MM 56: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V

Time: Thursday 15:00–18:15

Location: H24

MM 56.1 Thu 15:00 H24

Zero-point renormalization of the electronic structure: trends across chemical and structural space — ●HONGHUI SHANG¹, CHRISTIAN CARBOGNO¹, PATRICK RINKE^{1,2}, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — ²Aalto University, Helsinki, Finland

The importance of the renormalization of the electronic structure due to the zero-point nuclear motion (ZPR) has been discussed since long [1,2], but only recent advances in the first-principles treatment of electron-phonon coupling (EPC) enabled an accurate assessment of this effect for simple, prototypical materials, e.g., diamond [3] and Si [4]. However, it is largely unknown how chemical and structural properties affect the ZPR. To shed light on this question, we compute the EPC and ZPR for the octet binaries in both the zincblende and NaCl structure. Computationally, this is achieved by exploiting our recent implementation of density-functional perturbation theory in real-space, which provides considerable computational advantages with respect to numerical costs, parallelization, and especially scalability with respect to the number of atoms. We demonstrate the validity of our implementation by comparing with existing studies and finite difference results, investigate the trends across chemical/structural space, and critically discuss the role of the exchange-correlation functional.

- [1] P. B. Allen and V. Heine, *J. Phys. C* **9**, 2305 (1976).
- [2] M. Cardona, *Solid State Commun.* **133**,3 (2005).
- [3] F. Giustino, *et.al. Phys. Rev. Lett.* **105**, 265501 (2010).
- [4] S. Ponc e, *et.al. J. Chem. Phys.* **143**, 102813 (2015).

MM 56.2 Thu 15:15 H24

All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — ●CHRISTIAN VORWERK, CATERINA COCCHI, and CLAUDIA DRAXL — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

We present an all-electron approach of the many-body perturbation theory to describe X-ray absorption spectroscopy (XAS) in solid-state materials. In this formalism, the electron-hole interaction is explicitly included by solving the Bethe-Salpeter equation. A fully relativistic description of core states, as implemented in the all-electron full-potential code `exciting`[1], enables the explicit treatment of the effects of spin-orbit coupling in the spectra. We investigate the XAS for prototypical systems, such as TiO₂ and MgO, considering excitations from oxygen K and metal L edges. Our results, in good agreement with experiments, allow us to gain insight into the nature of the core-level excitations of these materials.

- [1] A. Gulans et al., *J. Phys. Condens. Matter* **26**, 363202 (2014).

MM 56.3 Thu 15:30 H24

Cohesive properties from all-electron RPA total energies — ●MARKUS BETZINGER¹, CHRISTOPH FRIEDRICH¹, ANDREAS GÖRLING², and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — ²Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

We present an all-electron implementation of the RPA total energy within the full-potential linearized augmented plane-wave (FLAPW) method. An incomplete basis-set correction (IBC) [1] is employed to improve the convergence of the total energy with respect to the basis-set and the number of unoccupied states. To some extent the IBC incorporates an infinite number of bands and enables a virtually exact treatment of the core electrons.

We demonstrate that the core electrons give rise to a sizeable contribution to the RPA total energy. Their individual contribution is comparable to that of the valence electrons. All-electron RPA lattice constants and bulk moduli are shown for a set of prototype materials and compared to experimental results. An excellent agreement with experiment is observed.

[1] M. Betzinger *et al.*, Phys. Rev. B (accepted, 2015); **88**, 075130 (2013); **85**, 245124 (2012).

MM 56.4 Thu 15:45 H24

Explicitly correlated self consistent field theory — ●CHRISTIAN LASAR and THORSTEN KLÜNER — Universität Oldenburg

Explicitly correlated correlation methods are an interesting field of current research since they are able to drastically improve the otherwise slow basis set convergence of conventional correlation methods. Therefore, chemical accuracy can be achieved with rather small basis sets.[1] The new correlation method presented in this contribution has already been developed for two-electron systems a long time ago[2]. We present the generalization of this ansatz to N-electron systems.

The basic idea is to augment a single Slater-determinant with an explicitly correlated prefactor which then takes care of the correlation effects and the basis set convergence. Another interpretation of this ansatz would be a contracted CISD with orbital optimization in a complete basis set. The contraction is achieved by the explicitly correlated prefactor whose choice therefore defines the possible accuracy of the method. In principle, the generalization to any pair method i.e. CCSD and MP2 will be possible.

The big advantage of this kind of ansatz for the wave function is the drastic reduction of matrix elements needed for the optimization of the wave function. As a result, the presented method will be applicable to large molecules.

[1] Chem. Rev. 112, p. 4 (2012) [2] J. Chem. Phys. 99, p. 8830 (1993)

MM 56.5 Thu 16:00 H24

Representing energy landscapes by combining neural networks and the empirical valence bond method — ●SINJA KLEES¹, RAMONA UFER², VOLODYMYR SERGIEVSKIY², ECKHARD SPOHR², and JÖRG BEHLER¹ — ¹Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — ²Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for large systems. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped by reference electronic structure calculations. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased. Preliminary results will be discussed and compared to density functional theory data.

MM 56.6 Thu 16:15 H24

CELL: a python package for cluster expansions with large parent cells — ●SANTIAGO RIGAMONTI¹, MARIA TROPPEZ¹, CHRISTOPHER SUTTON², LUCA M. GHIRINGHELLI², and CLAUDIA DRAXL¹ — ¹Humboldt-Universität zu Berlin — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft

The discovery of new materials for applications in areas such as energy harvesting, relies more and more on the accurate theoretical descrip-

tion of complex structures with large unit cells. The properties of interest are often tuned by substitutional dopants. Due to the vast configurational dopant space, a wide-spread approach is the cluster expansion (CE) technique. Most available CE codes are designed for alloys based on small parent cells, with usually 1 to 4 atoms. For the many important materials with much larger parent cells such approaches can't be applied. We devise an iterative scheme, based on efficient samplings of the configurational space, avoiding full structure enumerations. CELL consists of several modules that can be used independently, enabling to design CEs for specific purposes. Various CE schemes are available, offering ℓ_2 and ℓ_1 norms as penalization terms and different cross-validation strategies. Methods such as LASSO and split Bregman iteration are available for dealing with the ℓ_1 norm (compressive sensing). Access to finite-temperature properties and the characterization of phase transitions is possible through the Wang-Landau and diffusive nested sampling modules. Examples are presented for type-I thermoelectric clathrates, with 46 sites in the parent cell.

MM 56.7 Thu 16:30 H24

Structural and electronic properties of the thermoelectric clathrates Ba₈Al_xSi_{46-x} and Sr₈Al_xSi_{46-x} — ●MARIA TROPPEZ, SANTIAGO RIGAMONTI, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin

Clathrate compounds are promising candidates for high-efficiency thermoelectric applications. Their cage-like structure containing guest atoms allows for exploiting the idea of the phonon-glass electron-crystal and reaching a large figure of merit. We study Ba₈Al_xSi_{46-x} and Sr₈Al_xSi_{46-x} ($6 \leq x \leq 16$), where optimal electronic properties are expected close to the Zintl composition ($x = 16$). Cluster expansions on various quantities are performed, thus having access to ground-state as well as finite-temperature properties. A linear increase of the lattice constant with the number of Al substituents is obtained (0.019 Å per Al addition) confirming experimental observations (0.02 Å). The calculated bond distances between high-symmetry sites agree well with experiment for the full compositional range [1,2]. We find a close correlation between bond distances and fractional Al occupancies. This helps improving models used by experimentalists to estimate fractional occupancies. The substitutional configurations present an order-disorder transition around 600 – 900 K, which is further analyzed applying the Wang-Landau method. An important finding is the semiconducting behavior of the low-temperature ordered phase at the Zintl composition, which points out the technological relevance of these compounds.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)

[2] M. Bobnar *et al.*; *Dalton Trans.* **44**, 12680 (2015)

MM 56.8 Thu 16:45 H24

Ab-initio calculation of Raman spectra of graphene-based materials — ●ALBIN HERTRICH, CATERINA COCCHI, PASQUALE PAVONE, and CLAUDIA DRAXL — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering is an important non-destructive method for characterizing carbon-based materials. The main features of experimental Raman spectra of pristine graphene and graphite are the first-order G-band at $\approx 1580 \text{ cm}^{-1}$ and the dispersive second-order 2D-band at $\approx 2700 \text{ cm}^{-1}$. We calculate first- and second-order Raman spectra fully *ab-initio* using the full-potential all-electron DFT package exciting [1], which allows for the calculation of both phonon dispersion, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-Salpeter equation. In our approach [2], we expand the dielectric tensor with respect to the phonon normal coordinates. By taking its derivatives and by computing vibrational matrix elements, we calculate Raman scattering intensities. Applying this scheme to monolayer graphene, bilayer graphene, and graphite, we obtain the G-band in good agreement with experiment [3]. Furthermore, we explore the influence of both the stacking sequence and the laser energy on the 2D-band.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).

[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).

[3] A. C. Ferrari *et al.*, Phys. Rev. Lett. **97**, 187401 (2006).

MM 56.9 Thu 17:00 H24

Exciton dispersion in layered and 2D systems — ●FRANCESCO SOTTILE^{1,2}, GIORGIA FUGALLO^{1,2}, PIERLUIGI CUDAZZO^{1,2}, and MATTEO GATTI^{1,2,3} — ¹Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — ²European Theoretical Spectroscopy Facility

— ³Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

The study of the exciton dispersion is of paramount importance for all applications involving light harvesting, beside providing fundamental knowledge about exciton mobility and migration. Using state-of-the-art *ab initio* many-body approach, like the Bethe-Salpeter equation [1], we present a first principle study of exciton dispersions in layered materials and 2D systems. Results for the former systems (on the prototypical hBN and MoS₂) have been recently confirmed by experiments carried out at the Synchrotron ESRF [2]. For the latter (2D) systems we investigate exciton dispersion in graphane and hBN. From our results we provide a general picture of the mechanisms governing the dispersion of neutral excitations in 2D systems, and of the role played by the confinement of the electronic charge in setting the exciton binding energy. In particular we found that due to the strongly reduced screening of the Coulomb interaction in low-dimensional materials, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size [3]. [1] M. Gatti et al., *Phys. Rev. B* **88**, 155113 (2013) [2] G. Fugallo et al. *Phys. Rev. B* **92**, 165122 (2015) [3] P. Cudazzo et al. submitted to *Phys. Rev. Lett.*

MM 56.10 Thu 17:15 H24

Electronic structure of selected superheavy elements ($Z > 104$) — ●HANA CENCARIKOVA¹ and DOMINIK LEGUT² — ¹Institute of Experimental Physics, SAS, Kosice, Slovakia — ²IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

The electronic structure of selected super-heavy elements ($Z > 104$) have been determined from the first-principle calculations based on the density functional method. To determine the ground-state structure we have calculated number of basic phases including the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures. Our results were obtained using local density approximation for the exchange and correlation effects and without and with the spin-orbit interaction for the band states. The analysis has been focused on the determination of the electronic density of states, electronic band structure dispersion relation, mechanical properties (elastic constants) and selected thermodynamical properties.

MM 56.11 Thu 17:30 H24

Layer-resolved calculated vibrations at gold surfaces — ●ANDREI POSTNIKOV¹ and KAMIL MOLDOSANOV² — ¹Université de Lorraine, LCP-A2MC, Metz, France — ²Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Vibration modes at (001), (011) and (111) surface of gold are calculated from first principles, using the SIESTA method [1] and the frozen phonon approach. Calculations are done on thick slabs of moderate lateral size – (2×2) for (001), (2×3) for (011), (3×3) for (111). This allows to resolve the vibration patterns layer by layer into the depth, in dependence on the in-plane wavevector component, and discriminating the polarisation of vibration modes. One notes the softening of modes at the surface, and an appearance of specifically surficial modes. The bulk behaviour is largely recovered from the 5th or 6th layer downwards.

This study was driven by an intention to grasp the properties of longitudinal acoustic modes propagating at some depth under the surface of gold nanoparticles, which were an important element of our recent work related to the mechanism of radiofrequency absorption and hence resulting heating of nanoparticles of $\gtrsim 5$ nm size [2]. Since it is difficult to meaningfully incorporate the diversity of the nanoparticles' shapes in a practical calculation, the vibrations beneath the most common facets occurring at the nanoparticles' surface were studied instead.

1. The SIESTA method, <http://departments.icmab.es/leem/siesta/>.
2. A. Postnikov and K. Moldosanov, <http://arxiv.org/abs/1508.00735>.

MM 56.12 Thu 17:45 H24

Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — ●ZUZANA GROSMANOVA¹ and DOMINIK LEGUT² — ¹Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — ²IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

In this work, the mechanical (elastic constants) and thermodynamic properties of actinium were investigated using first-principle calculations. Our results were obtained using density functional theory employing local density and general gradient approximation for the electronic exchange-correlation effects and including the spin-orbit interaction for the band states. The ground-state structure were determined among simple phases like the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures.

MM 56.13 Thu 18:00 H24

Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — ●CHRISTOPH LECHNER¹, PHILIPPE BARANEK¹, and HOLGER VACH² — ¹EDF Lab Les Renardières, Avenue des Renardières, F-77818 Moret-sur-Loing Cedex, France — ²CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine 36. Therefore, a computational study of the interaction of tritium and chlorine 36 with defects in graphite has been achieved at the density functional theory (DFT) level by using the functionals PBE and PBE0 with Grimme's D3 dispersion correction. The physisorption and chemisorption of atomic and molecular hydrogen or chlorine on graphite surfaces, (001), (100), and (110) with or without mono- and divacancies, have been investigated. The stabilities of the formed complexes are interpreted in terms of the formation energy. To obtain insight into the nature of the bonding a population analysis of the systems has been performed. While the bonding of hydrogen is mostly covalent for chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Raman spectra for selected structures have been investigated, in order to evaluate, if the experimentally observed defect bands can be reproduced.

MM 57: Invited talk Markmann

Time: Thursday 15:00–15:30

Location: H38

Invited Talk MM 57.1 Thu 15:00 H38

Virtual diffraction as a tool to investigate nanostructured materials — ●JÜRGEN MARKMANN — Helmholtz-Zentrum Geesthacht, Institut für Werkstofforschung, Werkstoffmechanik, Geesthacht, Germany — Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie, Hamburg, Germany

The boost in computational resources during the last years caused a considerable increase in simulation studies of materials on the atomistic scale. Several tools for detailed local analyses have been developed but they usually leave the difficulty of transferring the gained knowledge into macroscopically measurable data. Knowing the exact position of the mass centres (atoms or grid points) of a material allows the calculation of its wide-angle and small-angle diffraction pattern. Tak-

ing into account all experimental artefacts, these virtual diffraction patterns can be analysed in an identical way one would do it in a laboratory experiment. A modification of the method also makes direction dependent investigations possible. Shown here are findings revealed by application of this method on MD simulated nanocrystalline palladium during deformation and the first tries to apply this method to nanoporous gold. Among other things, an intrinsic nature of microstrain in nanocrystalline materials was discovered and the contribution of grain boundaries to the elastic deformation of nanocrystalline materials was illustrated.

- [1] Markmann, Yamakov, Weissmüller, *Scripta Mater.* **59** (2008) 15.
- [2] Markmann, Bachurin, Shao, Gumbsch, Weissmüller, *Europhys. Lett.* **89** (2010) 66002.

MM 58: Biomaterials and Biopolymers III (Joint Session with CPP/BP/MM)

Joint session with CPP and MM organized by BP.

Time: Thursday 15:00–16:15

Location: H45

MM 58.1 Thu 15:00 H45

Contribution of Biofilm Matrix Components to Physical Material Properties of Bacterial Biofilms — ●SARA KESEL, STEFAN GRUMBEIN, INA GÜMPERLEIN, ANNA-KRISTINA MAREL, MARWA TALLAWI, OLIVER LIELEG, and MADELEINE OPITZ — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Bacteria can be protected from antibiotics, chemicals and mechanical stresses by a self-produced matrix, the so called biofilm. As biofilms can grow on various surfaces such as medical implants, this poses a big problem in health care and industry. Biofilm matrices can thereby consist of different extracellular substances (EPS) such as polysaccharides, proteins, lipids and nucleic acid. Understanding of the individual contributions to the above described resistances by the different biofilm matrix components is therefore necessary, in order to prevent and fight biofilm growth. In particular, it is important to understand at what stage of biofilm formation the observed resistances are developed. In this study, different stages of biofilm growth (attachment of single cells, microcolony growth, as well as mature biofilms) were investigated using several techniques such as e.g. cantilever arrays, time-lapse microscopy and atomic force microscopy. The attachment of single bacteria onto solid surfaces and further physical material properties of two *B. subtilis* wild-type strains that differ in their biofilm matrix composition were analyzed. Furthermore, using several mutant strains the impact of specific biofilm matrix elements on the observed biofilm properties was quantitatively analyzed.

MM 58.2 Thu 15:15 H45

Multiple bio-functionalization in 3D-scaffolds for cell manipulation realized by orthogonal (photo)chemistry — ●VINCENT HAHN¹, BENJAMIN RICHTER², TANJA CLAUS^{3,4}, GUILAUME DELAITTRE^{3,5}, CHRISTOPHER BARNER-KOWOLLIK^{3,4}, MARTIN WEGENER^{1,6}, and MARTIN BASTMEYER² — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT) — ²Zoological Institute and Institute for Functional Interfaces, KIT — ³Institute for Chemical Technology and Polymer Chemistry, KIT — ⁴Institute for Biological Interfaces, KIT — ⁵Institute for Toxicology and Genetics, KIT — ⁶Institute of Nanotechnology, KIT

In recent years, we have applied Direct Laser Writing to fabricate 3D-microscaffolds for culturing cells in a well-defined environment and investigated cellular responses, e.g., contractility, adhesion and shape.

By sequential writing of different photoresists, patterned scaffolds are realized. They consist of protein-binding polymers next to regions containing light-activatable monomers in a non-protein binding background. Upon light-activation we were able to biotinylate specific regions in the passivating backbone. When incubated with a protein solution, proteins adsorb only onto protein-binding polymer areas. The biotin-linker is subsequently addressed by using avidin and any other biotinylated protein of choice. This technique has been successfully applied to fabricate scaffolds functionalized with two different adhesion proteins that selectively direct cell adhesion.

Such scaffolds might prove useful for applications in tissue engineering and stem cell differentiation.

MM 58.3 Thu 15:30 H45

Different protein adsorption rates on different grain orientations in hydroxyapatite — ●THOMAS FAIDT, JÖRG SCHMAUCH, MICHAEL DECKARM, SAMUEL GRANDTHYLL, FRANK MÜLLER, and KARIN JACOBS — Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken

As a model system for tooth enamel, hydroxyapatite (HAP) pellets with a density of > 97% of the theoretical crystallographic density of

HAP have been produced by compacting and sintering commercially available HAP powder. Atomic force microscopy (AFM) combined with electron backscatter diffraction (EBSD) measurements reveal the smoothness and the crystal orientation of the HAP grains on the surface of the pellets. On these surfaces, single molecule BSA adsorption experiments are performed in a microfluidic setup and reveal that different grain orientations provoke different adsorption rates. These findings open a pathway to control protein adsorption.

MM 58.4 Thu 15:45 H45

Studying Biomineralization with ultrathin silica sheets grown at the air-water interface. — ●HELMUT LUTZ¹, VANCE JAEGER², RÜDIGER BERGER¹, MISCHA BONN¹, JIM PFAENDTNER², and TOBIAS WEIDNER¹ — ¹Max Planck Institute for Polymer Research Ackermannweg 10, Mainz 55128, Germany — ²Chemical Engineering University of Washington 105 Benson Hall, Seattle, WA 98195-1750, USA

Inspired by diatom silification we used amphiphilic peptides consisting of leucine and lysine (LK peptides) to investigate biomineralization at surfaces. Depending on hydrophobic periodicity, these peptides adopt alpha helical or beta sheet structures at the air-water interface. Upon addition of a silica precursor we obtained surface-tailored peptide-silica hybrid films with a thickness of ~4 nm. We probed film composition and interactions between peptides and silica at early stages of biomineralization by means of surface sensitive techniques, such as sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS). Electron and atomic force microscopy show similarities of the film fine structure and the surface of in-solution silica precipitates. Experimental findings were complemented with molecular dynamics simulations. We believe that our results provide insights into the biomineralization of structured films, which might prove useful in materials design and surface engineering.

H. Lutz, V. Jaeger, R. Berger, M. Bonn, J. Pfaendtner, T. Weidner, *Advanced Materials Interfaces* 2015, 2, n/a. J. E. Baio, A. Zane, V. Jaeger, A. M. Roehrich, H. Lutz, J. Pfaendtner, G. P. Drobný, T. Weidner, *Journal of the American Chemical Society* 2014, 136, 15134.

MM 58.5 Thu 16:00 H45

AFM force spectroscopy with *S. aureus* and *Strep. mutants* to reveal biopolymer binding properties — ●FRIEDERIKE NOLLE¹, NICOLAS THEWES¹, CHRISTIAN SPENGLER¹, KORDULA SCHELLNHUBER¹, PETER LOSKILL¹, ALEXANDER THEWES², LUDGER SANTEN², and KARIN JACOBS¹ — ¹Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken — ²Saarland University, Dept. of Theoretical Physics, 66041 Saarbruecken

The adhesion of pathogenic bacteria is a crucial step in the development of implant-related infections. The adhesion of bacteria is mediated by biopolymers, the properties of which we are able to characterize by AFM force spectroscopy, where the probe is a single bacterium. To deepen the understanding, we combine the AFM studies with computer simulations [1]. For bacteria (*Staphylococcus aureus*) in contact with hydrophobic surfaces, thermally fluctuating cell wall proteins of different stiffness attach to the surface via short range forces and subsequently * due to entropic forces * pull the bacterial cell into close contact. That way, *S. aureus* is able to substantially increase its interaction range for contact initiation. Bacteria like *Streptococcus* mutants also attach to hydrophilic surfaces (e.g. titanium or hydroxyapatite) in the presence or absence of other biomolecules (proteins, enzymes). Our study reveals the importance of specific parameters (e.g. roughness) and proposes that fluctuations in protein density and structure are much more relevant than the exact form of the binding potential.

[1] N. Thewes, P. Loskill, P. Jung, H. Peisker, M. Bischoff, M. Herrmann, K. Jacobs, *Soft Matter* 2015, 11, 8913-8919

MM 59: Topical session: In-situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science VII - Nanomaterials

Time: Thursday 15:45–18:30

Location: H38

MM 59.1 Thu 15:45 H38

In situ off-axis electron holography of magnetic nanoparticles — ●RAFAL E. DUNIN-BORKOWSKI, ANDRÁS KOVÁCS, and JAN CARON — Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany

Off-axis electron holography is a powerful technique for recording the phase shift of a high-energy electron wave that has passed through an electron-transparent specimen in the transmission electron microscope. The phase shift is, in turn, sensitive to the electrostatic potential and magnetic induction in the specimen, projected in the electron beam direction. We are currently using the technique to characterize the magnetic properties of individual and closely-spaced deep-submicron-sized nanoparticles, nanostructures and thin films that are subjected to externally applied magnetic fields in situ in the transmission electron microscope, as well as to elevated and reduced temperature. We are also working on a model-based approach that can be used to reconstruct the three-dimensional magnetization distribution in a specimen from a series of phase images recorded as a function of specimen tilt angle using off-axis electron holography. We make use of a forward simulation approach within an iterative model-based algorithm to solve the inverse problem of reconstructing the three-dimensional magnetization distribution in the specimen from tilt series of two-dimensional phase images recorded about two independent tilt axes. In such applications of off-axis electron holography, the effects of electron beam induced charging and dynamical diffraction should be minimized.

MM 59.2 Thu 16:15 H38

Encapsulated silver nanowire electrodes: applications, computer based analysis and stability tests — ●MANUELA GÖBELT¹, RALF KEDING¹, MATTHIAS BÜCHELE¹, BJÖRN HOFFMANN¹, and SILKE CHRISTIANSEN^{1,2} — ¹Max-Planck-Institute for the Science of Light, Erlangen, Germany — ²Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany

Transparent electrodes are a critical component in optoelectronic devices like solar cells. We developed a novel nano-composite transparent electrode material composed of a wet-chemically synthesized silver nanowire (AgNW) network encapsulated in a transparent conductive oxide which was deposited with nano-scale precision by atomic layer deposition. To demonstrate the performance of the AgNW/AZO electrode, it was used as a top electrode on different optoelectronic devices. With a combination of scanning electron microscopy images and computer based image analysis we can characterize the AgNW networks and determine the percolation of them on large areas. For the object recognition "ImageJ" serves as a basis and a combination of existing plugins and self-written software is used. The new software is capable of handling high aspect ratio objects in an interconnected network, where every single object has several intersections with others. It is possible to distinguish the single wires and to reconstruct their original shape although they are partly covered by others objects. We also take a detailed look at the stability of these nano-composite electrodes under ambient conditions and we will show how the AZO encapsulation shelters the AgNW networks from oxidation and sulfurization.

MM 59.3 Thu 16:30 H38

Structural and optical investigation of colloidal gold platelets for high-quality plasmonic applications — ●BJÖRN HOFFMANN¹, MUHAMMAD BASHOUTI¹, THORSTEN FEICHTNER^{2,1}, MIRZA MAČKOVIĆ³, CHRISTEL DIEKER³, AHMED SALAHELDIN⁴, PETER RICHTER⁵, OVIDIU GORDAN⁵, DIETRICH ZAHN⁵, ERDMANN SPIECKER³, and SILKE CHRISTIANSEN^{2,1} — ¹Max Planck Institute for the Science of Light, 91058 Erlangen — ²Helmholtz Zentrum Berlin für Materialien und Energie GmbH, D-14109 Berlin — ³Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Mikro- und Nanostrukturforschung (WW9) & Center for Nanoanalysis and Electron Microscopy, Department Werkstoffwissenschaften, 91058 Erlangen — ⁴FAU Erlangen-Nürnberg, Institute of Particle Technology, 91058 Erlangen — ⁵Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz

Wet-chemically synthesized ultraflat gold platelets are an ideal building block for high-quality plasmonic applications. They show superior

properties compared to vapor-deposited gold layers and enable yet unknown fabrication precision. Even though gold platelets are already frequently used in the field of plasmonics, many details about their intrinsic structure as well as their optical properties are still unknown.

Here, we present a detailed TEM study that proves the existence of twin boundaries inside the particles. Furthermore, we have determined the complex dielectric function of single gold platelets by using micro-ellipsometry. To demonstrate the outstanding quality of this material, we prepared ultrathin, single-crystalline layers as thin as 15 nm.

MM 59.4 Thu 16:45 H38

The role of CTAB micelles in gold nanorod synthesis - a combined SAXS/SANS study — ●TILO SCHMUTZLER, TORBEN SCHINDLER, and TOBIAS UNRUH — Friedrich-Alexander-University Erlangen-Nuernberg, Chair for Crystallography and Structural Physics, Staudtstrasse 3, 91058 Erlangen, Germany

Au nanoparticles have been the subject of widespread research in the last two decades. Applications are expected in biological imaging, drug delivery and phototherapeutics.

The common wet chemical synthesis of gold nanorods (AuNRs) is the seed-mediated growth synthesis route.[1] Therefore small seed particles are used to grow nanorods in a solution of CTAB (Cetyltrimethylammonium bromide) as structure directing agent.

The behaviour of CTAB in solution and so the influence on the final AuNR formation can be influenced by additives like inorganic salts. Increasing concentrations of KBr for example lead to a slower formation kinetic of AuNRs which was investigated by time-resolved small angle X-ray scattering (SAXS) simultaneously to UV-Vis spectroscopy. Additionally the rod formation beside other morphologies is less pronounced compared to the synthesis in solutions without further KBr. The influence of CTAB as catalytically active component is obvious due to the change of the scattering related to the micelles itself. Therefore small angle neutron scattering (SANS) is perfectly suitable to analyze the structure of CTAB modified by different additives to understand the behavior during AuNR formation.

[1] C.J. Murphy et. al, J. Phys. Chem B. 2005, 109, 13857-13870.

15 min. coffee break

MM 59.5 Thu 17:15 H38

In Situ Methods for Studies of Mechanically, Thermally, Electron Beam and Liquid Induced Effects in Nanostructured Materials — ●EVA OLSSON — Chalmers University of Technology, Göteborg, Sweden

In situ electron microscopy allows the imaging of transport of matter and charges in complex structures as well as heat spread. We can study mechanically and thermally induced changes of charge transport properties using holders designed to enable different stimuli allowing the direct observation and correlation between material structure and properties. This talk addresses examples of in situ mechanical, thermal and liquid studies. We have studied the effect of mechanical strain on the electrical resistance of nanowires. Electron energy loss spectroscopy was used to study the effect of strain on the electronic structure with emphasis on the low energy loss interval of 0 to 50 eV. Electron beam induced current measurements were also performed to study the effect of strain on the diffusion length of the charge carriers. Heating of a transmission electron microscopy specimen can be performed in several parallel modes and this talk will address three types of heating modes and show experimental results from nanostructured materials. The talk will also show a technique for in situ wetting of materials in the environmental scanning electron microscope and applied it to suspended coatings. The method uses a manipulator to bring the specimen in contact with a water reservoir in the microscope chamber and provides direct visual information about the water interaction with the material at a high spatial resolution.

MM 59.6 Thu 17:45 H38

Interaction of commensurate charge density waves with ionic point defects in electron beam irradiated 1T-TaSe2 and 1T-TaS2 — ●MICHAEL KINYANJUI^{1,2}, PIA KYNRIM², TIBOR LEHNERT², JANIS KOSTER², and UTE KAISER² — ¹Helmholtz Institute

Ulm, Helmholtzstraße 11, 89081 Ulm, Germany — ²Central Facility of Electron Microscopy, Ulm University, Albert Einstein Allee 11, 89068 Ulm, Germany

Low dimensional transition metal dichalcogenides (MX₂, M = transition metal e.g Nb, Mo, Ti X= chalcogen e.g S, Te, Se) are of great interest due to some of their unique properties including metal-insulator transitions and charge density waves (CDW) observed as a function of temperature, pressure, and doping. Here we report on the interaction of commensurate charge density waves and anionic point defects in 1T-TaSe₂ and 1T-TaS₂. By using atomic resolved high resolution transmission microscopy (HRTEM) we show the loss of CDW long range order as a result of the interaction with S and Se vacancies generated by the electron beam irradiation. We discuss the loss of long range order as a result of the interaction between the CDW and the Friedel oscillations arising from the point defects.

MM 59.7 Thu 18:00 H38

X-ray Nanodiffraction for in situ Microscopy — ●CHRISTINA KRYWKA^{1,2}, STEPHAN V. ROTH³, and MARTIN MÜLLER¹ — ¹Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht — ²Christian-Albrechts-Universität, Leibnizstraße 19, D-24118 Kiel — ³DESY, Notkestraße 85, D-22607 Hamburg

The origins of the macroscopic behavior of synthetic and natural high-performance materials can often be found on no less than atomistic length scales. Access to these dimensions is barred for light microscopes while electron microscopes suffer from the low penetration depth of electrons. Consequently, high resolution structural data recorded with external stimuli modified *in situ* is rare to find. X-ray nanodiffraction is able to overcome these hurdles. That's because a sub-micrometer sized hard X-ray beam can extract local structural information residing within bulk volumes and from samples inside extended sample environments - given a sufficiently long focal distance. The Nanofocus Endstation of P03 beamline (PETRA III) is a dedi-

cated X-ray nanodiffraction setup. Tensile and indentation stresses, magnetic and electric fields, hydrostatic pressure and fluid shear have all been applied *in situ* in past nanodiffraction experiments at P03, i.e. while high resolution structural information data were recorded. Not only do these results emphasize our focus on materials science but they also demonstrate why X-ray Nanodiffraction is a genuine *in situ* microscopy technique.

MM 59.8 Thu 18:15 H38

A setup for AFM-based pick-and-place handling of nano-objects inside an SEM — ●UWE MICK^{1,2}, PETER BANZER^{1,2,3}, SILKE CHRISTIANSEN^{1,4}, and GERD LEUCHS^{1,2,3} — ¹Max Planck Institute for the Science of Light, Erlangen, Germany — ²Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Erlangen, Germany — ³Max Planck - University of Ottawa Centre for Extreme and Quantum Photonics, Ottawa ON, Canada — ⁴Institute of Nano-Architectures for Energy Conversion, Helmholtz-Zentrum Berlin, Berlin, Germany

Employing AFM technology for nanomanipulation is well-established. However, as a stand-alone technology, the AFM lacks immediate visual feedback on the manipulation in progress. Here we present a Dual-AFM system that is integrated into an SEM and dedicatedly designed to enable pick-and-place handling of nano-objects under the in-situ visual control of the SEM. Several usage scenarios for handling nanowires and nanoparticles down to below 100 nm in diameter are shown; including general schemes for adapting the shape of AFM probe tips by FIB milling to specific manipulation tasks. As the main application, the prototyping of plasmonic particle patterns is presented and specifically the capability to select building blocks from different sources to fabricate heterogeneous nanoparticle patterns. When preparing glass samples for photonic applications in an SEM, additional challenges arise. Therefore, a toolchain of methods and instruments for pre-characterizing and selecting suitable nano-building-blocks and mitigating charging effects during sample preparation are outlined.

MM 60: Microstructure and Phase Transformations III

Time: Thursday 15:45–17:00

Location: H39

MM 60.1 Thu 15:45 H39

Mechanically driven BCC to BCT phase transformation during wire drawing conditions of pearlitic steel: An ab initio guided model — ●GH. A. NEMATOLLAHI¹, S. DJAZIRI¹, Y. LI¹, C. KIRCHLECHNER¹, B. GRABOWSKI¹, S. GOTO^{1,2}, D. RAABE¹, G. DEHM¹, and J. NEUGEBAUER¹ — ¹Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany — ²Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-8502, Japan

Cold-drawn pearlitic steel wires revealing ultra-high tensile strengths of up to 7 GPa are the world's strongest bulk materials. Experimental observations reveal that cementite gradually decomposes during wire drawing. The C atoms resulting from the cementite decomposition are mechanically alloyed into the ferrite phase and accommodated in trapping sites around defects, such as dislocations. Surprisingly, there is also a high oversaturation of the bulk ferrite phase and experiments indicate a transformation to a tetragonally distorted system. In this work, a new ab initio informed model has been developed to take into account the strain-induced interaction of C with the host matrix as characteristic for wire drawing conditions. Our model captures the effect of the applied strain * exerted by the wire drawing process * within a renormalized C formation energy obtained by density functional theory calculations. Applying the model we demonstrate that the experimentally observed tetragonal distortion is due to a mechanically driven phase transformation from the body-centered-cubic (bcc) to the body-centered tetragonal (bct).

MM 60.2 Thu 16:00 H39

First-principle study of phase transformations in Ni₂MnGa alloy — ●MARTIN ZELENÝ^{1,2}, ALEXEI SOZINOV³, LADISLAV STRAKA⁴, and OLEG HECKZO⁵ — ¹Institute of Materials Science and Engineering, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — ²Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — ³Material Physics Laboratory, Lappeenranta University of Technology, Savonlinna, Finland — ⁴Aalto University School of

Engineering, Laboratory of Engineering Materials, Aalto, Finland — ⁵Institute of Physics of Academy of Sciences of the Czech Republic, Prague, Czech Republic

Transformation path between different phases of Ni₂MnGa alloy has been investigated using first-principle electronic structure calculations. We used the projector-augmented wave method for the calculations of total energies and stresses along the transformation paths. These include transformation from austenite (A) to nonmodulated tetragonal martensite (NM), transformation from modulated martensites (10 M and 14 M) to NM martensite, as well as transformation between adjacent twin variants of NM phase. All transformations are induced by applying external shear strain. The results show the same barrier equal to 0.4 mRy/atom for A→NM transformation, 10M→NM transformation and NM twin reorientation whereas 14M→NM transformation exhibits smaller barrier equal to 0.25 mRy/atom. Calculated lower barrier well corresponds to experimental finding that the transformation from 10M to NM always proceeds via intermediate 14M phase.

MM 60.3 Thu 16:15 H39

Martensitic phase transformation of Fe₇₀Pd₃₀ ferromagnetic shape memory alloy thin films due to laser shock peening — ●ALINA J. BISCHOFF¹, ARIYAN ARABI-HASHEMI¹, MARTIN EHRHARDT¹, PIERRE LORENZ¹, KLAUS ZIMMER¹, and STEFAN G. MAYR^{1,2} — ¹Leibniz-Institut für Oberflächenmodifizierung, Leipzig — ²Fakultät für Physik und Geowissenschaften, Universität Leipzig

The fcc-fct martensitic phase transformation induced by laser shock peening is analyzed in Fe₇₀Pd₃₀ ferromagnetic shape memory alloy thin films. At shockwave pressures of up to 2.5 GPa, X-ray diffraction and scanning electron microscopy measurements reveal formation of martensitic variants with preferred orientation of the shorter c-axis perpendicular to the surface plane. Consequential merging of growth islands on the film surface is observed. For a better understanding of the atomistics of these findings, twin boundary formation, which is characteristic of martensitic transition, as well as material shape change are further explored by classical molecular dynamics simula-

tions.

MM 60.4 Thu 16:30 H39

Density functional theory investigation of elastic properties and martensitic transformation of Ti-Ta alloys — ●TANMOY CHAKRABORTY, JUTTA ROGAL, and RALF DRAUTZ — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr- Universität Bochum, 44780 Bochum, Germany

Ti-Ta alloys are considered as promising materials for high temperature shape memory alloys as well as biomedical applications. The properties of these alloys have been shown to be strongly composition dependent. The temperature for the martensitic transformation between the high temperature cubic austenite and the low temperature orthorhombic martensite decreases linearly with increasing Ta content. Likewise, the elastic properties show clear trends with changing composition. We use density functional theory to investigate the involved phases in Ti-Ta where the disordered phases are treated by special quasi-random structures. To compare the stability of the involved phases as a function of temperature we calculate free energies using the quasi-harmonic Debye model. The obtained trends in the stability are consistent with experimentally measured transformation temperatures. Furthermore, we determine elastic properties which are in good agreement with experimentally observed trends.

MM 60.5 Thu 16:45 H39

Formation of interface layers in dissimilar Al-Cu FSW-Joints — ●ROLAND MARSTATT¹, MARKUS KRUTZLINGER², JOHANNES LUDERSCHMID¹, FERDINAND HAIDER¹, and MICHAEL F. ZAEH² — ¹Lehrstuhl fuer Experimentalphysik I, Universitaet Augsburg, Germany — ²Institut fuer Werkzeugmaschinen und Betriebswissenschaften, Technical University of Munich, Garching, Germany

Friction Stir Welding (FSW) is a suitable technology to join dissimilar materials, in contrast to fusion welding processes without exceeding the solidus temperature. As a consequence, high quality joints can be produced with a minimum of deleterious intermetallic phases. Due to the process conditions, FSW seems to be a good choice to form dissimilar joints as e.g. between aluminium and copper. Process optimization aims on high quality dissimilar joints with a minimum of deleterious intermetallic phases. But still an intermetallic layer at the bonding interface is detected. However, a comprehensive description of the effective joining mechanisms is still a subject of ongoing research.

In this study the analysis of the formation of nano-scaled intermetallic layers at the bonding interface is presented. These layers play a key role for the joining mechanism and influence mechanical properties and conductivity. Therefore, dissimilar lap joints of aluminium and copper with the pin stirring in aluminium only have been investigated. The thickness of the intermetallic layer highly depends on the process temperature which varies with different process parameters. Understanding the relevant process parameters for the formation of the interlayer allows to control the joint quality. *Supported by the DFG (SPP1640).*

MM 61: Functional materials IV: Batteries III

Time: Thursday 15:45–16:45

Location: H52

MM 61.1 Thu 15:45 H52

From micro- to mesoscale: The impact of occupational disorder on Li ion mobility in Li₄Ti₅O₁₂ battery materials — ●HENDRIK H. HEENEN, CHRISTOPH SCHEURER, and KARSTEN REUTER — Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Spinel-type lithium-titanium-oxide (Li₄Ti₅O₁₂) is an extraordinarily safe and long-living anode material employed in commercial lithium ion batteries. To complement experimental investigations, first-principles studies are often applied to gain microscopic insight into the underlying ion transport processes and the microscopic structure. This computationally demanding approach is however challenged by the treatment of the mixed occupancy of octahedral sites by Li and Ti ions found in Li₄Ti₅O₁₂. The resulting vast configuration space is usually reduced to an idealized model, oversimplifying the investigated system. A numerically efficient, yet reliable, classical interatomic potential [1], allows for exploring the complex configuration space through extensive Monte-Carlo sampling and evaluating its electrochemical properties via molecular dynamics simulations. Our findings indicate a higher Li ion mobility with structural disorder, which is thermodynamically favored by high synthesis temperatures. We further assess the Markovian processes of the diffusion mechanism via a thorough microscopic analysis and elucidate the Li ion mobility in detail. This yields dynamic rates necessary for an extrapolation to kinetic Monte-Carlo simulations which pave the way for more quantitative predictions.

[1] M. Vijayakumar *et al.*, *J. Power Sources* **196**(4), 2211 (2011);

MM 61.2 Thu 16:00 H52

Characterization of an all solid-state thin-film battery — ●SUSANN NOWAK¹, FRANK BERKEMEIER², and GUIDO SCHMITZ¹ — ¹Heisenbergstr. 3, 70569 Stuttgart — ²Corrensstraße 46, 48149 Münster

In this talk an all solid-state thin-film battery is shown, which has been produced by ion beam sputtering of all parts, featuring LFP as the cathode material, LiPON as the solid electrolyte and tin as the anode material. The battery is characterized by means of cyclic voltammetry (CV), chronopotentiometry (CP) and transmission electron microscopy (TEM). From these measurements the capacity and its dependence on the cycle number is determined. Measurements at different scan rates (CV) and comparison of the peak currents yield kinetic information, which are compared to the parameters of the individual materials. In contrast to conventional battery cells, solid-state batteries can be operated at elevated temperatures. Experiments under variation of temperatures demonstrate that the capacity of the

cell is significantly dependent on the temperature at which the cell is operated, pointing to a capacity loss due to kinetic restraints at room temperature. The obtained capacity after 100 cycles is starting at 20% of the LFP capacity (RT) and reaching 80% at 80°C. In contrast in a liquid cell the maximum capacity is already reached at room temperature.

MM 61.3 Thu 16:15 H52

Is it possible to achieve an all-solid-state thin-film Li-ion battery by laser assisted chemical vapor deposition (LA-CVD)? — ●CHRISTOPH LOHO¹, AZAD DARBANDI^{1,2}, RUZICA DJENADIC^{1,3}, OLIVER CLEMENS^{1,2}, and HORST HAHN^{1,2,3} — ¹Joint Research Laboratory Nanomaterials, Darmstadt, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — ³Helmholtz Institute Ulm, Ulm, Germany

Over the last decades a progressive miniaturization of electronic components took place. As a result there is an increasing demand for micro-sized power sources. In this respect an all-solid-state thin-film battery is desirable, since its excellent safety properties and easy integration in microelectronics are outstanding advantages. Furthermore, in the case of the garnet solid state electrolyte Li₇La₃Zr₂O₁₂, high voltage cathode materials and a lithium metal anode can be used to increase the energy density.

Chemical vapor deposition (CVD) is a suitable method to grow functional thin-films for Li-ion batteries, since it allows for homogeneous growth over large areas with high deposition rates and very high purity. Unique is also the capability of conformal, directional deposition in order to realize three-dimensional (3D) architectures.

In this contribution the successful deposition of LiCoO₂ on different 3D architectures is reported. In addition, it is shown that the Li-ion conductivity of Li₇La₃Zr₂O₁₂ thin-films deposited by LA-CVD exceeds 10⁻⁶ S/cm. Finally, the assembly of an all-solid-state thin-film Li-ion battery is discussed.

MM 61.4 Thu 16:30 H52

LiMn₂O₄ as a thin-film battery electrode material — ●JULIANE MÜRTER, SUSANN NOWAK, and GUIDO SCHMITZ — Institute of Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany

LiMn₂O₄ is a highly investigated cathode material for Li-ion batteries due to its low cost, low toxicity, and high voltage of over 4 V vs. Li. In this study, the material is deposited by ion-beam sputtering, with thicknesses ranging from 55 nm to 300 nm. Different post-deposition treatments are performed and the influence on capacity, cycle stabil-

ity, and rate capability is studied. Excellent cycling stability over 500 cycles with almost no loss in capacity is achieved. X-ray diffraction (XRD) is used to determine the crystal structure. The electrochemical performance is investigated using chronopotentiometry (CP) as well as cyclic voltammetry (CV).

Owing to the thin film geometry, the CV scan rate can be varied over 5 orders of magnitude presenting a consistent variation of peak current and overpotential. Using this data, experimental values are compared to kinetic models to determine the Li diffusion coefficient and the transfer coefficient through the surface.

MM 62: Methods in Computational Materials Modelling IV: Method development

Time: Thursday 15:45–17:45

Location: H53

MM 62.1 Thu 15:45 H53

Functional renormalization and mean-field approach to multi-band systems with spin-orbit coupling: Application to the Rashba model with attractive interaction — GIULIO SCHOBER¹, ●KAY-UWE GIERING¹, MICHAEL SCHERER¹, CARSTEN HONERKAMP², and MANFRED SALMHOFER¹ — ¹Heidelberg University — ²RWTH Aachen University

The functional renormalization group (RG) in combination with Fermi surface patching is a well-established method for studying Fermi liquid instabilities of correlated electron systems. In this article, we further develop this method and combine it with mean-field theory to approach multi-band systems with spin-orbit coupling, and we apply this to a tight-binding Rashba model with an attractive local interaction. The spin dependence of the interaction vertex is fully implemented in a RG flow without SU(2) symmetry, and its momentum dependence is approximated in a refined projection scheme. In particular, we discuss the necessity of including in the RG flow contributions from both bands of the model, even if they are not intersected by the Fermi level. As the leading instability of the Rashba model, we find a superconducting phase with a singlet-type interaction between electrons with opposite momenta. While the gap function has a singlet spin structure, the order parameter indicates an unconventional superconducting phase, with the ratio between singlet and triplet amplitudes being plus or minus one on the Fermi lines of the upper or lower band, respectively. We expect our general approach to be useful for an unbiased theoretical description of the low-temperature properties of spin-based materials.

MM 62.2 Thu 16:00 H53

Advanced Brillouin zone sampling for first-principles calculations — ●PHILIP HASNIP and MATTHEW PROBERT — University of York, York, UK

In quantum mechanical materials models such as density functional theory (DFT), the material's wavefunction is expressed as a Bloch function multiplied by a phase factor $\exp\{ik \cdot r\}$, where k is drawn from the material's first Brillouin zone. Solutions to the quantum equations exist for all k and many quantities, including the total energy, require an integration over all k ; these integrals are performed numerically on a finite mesh of sampling 'k-points'.

The sampling density required for accurate integration cannot be known a priori, and varies from material to material; metallic states require particularly high k-point densities in order to reproduce the Fermi surface accurately, yet metallicity is an emergent property of the simulation and cannot be known reliably beforehand.

In this work we discuss the common methods for performing this k-point integration, highlighting the problems encountered in real simulations, and present alternative methods which ameliorate these difficulties. In particular we present a fast estimate for the k-point sampling error which may be used dynamically to guide simulations. The method will be illustrated with results using the Castep DFT program.

MM 62.3 Thu 16:15 H53

The electronic structure of transition metal phthalocyanines: the influence of electron correlation — ●IULIA EMILIA BRUMBOIU, SOUMYAJYOTI HALDAR, JOHANN LÜDER, OLLE ERIKSSON, HEIKE C. HERPER, BARBARA BRENA, and BIPLAB SANYAL — Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden

Transition metal phthalocyanines (TMPcs) have been in the focus of scientific research as possible candidates for applications in spintronics and molecular electronics. These types of applications make use of the molecular spin and usually involve the adsorption of the TMPc on various substrates. In the framework of density functional theory, the description of the molecule adsorbed on a surface is not straightforward, especially due to the presence of the metal d electrons. A

compromise between accuracy and computational cost is achieved by combining DFT with a Hubbard term exclusively acting on the correlated electrons. Many studies on TMPcs adsorbed on surfaces make use of this approach, but the choice of U is mainly based on previously reported values for similar systems. We provide a detailed analysis of the influence of U on the electronic structure of five TMPcs (Mn-, Fe-, Co-, Ni- and CuPc). By comparing the calculated valence band to photoelectron spectra and by computing the Hubbard term from linear response, we show that U is different for every phthalocyanine. For each molecule, we provide a range of U values that show good agreement with the experiments. These values represent a safe starting point for DFT+ U calculations of physisorbed TMPcs.

MM 62.4 Thu 16:30 H53

Hybrid-functional calculations of iron defects in ferropericlase — ●SEBASTIÁN ALARCÓN VILLASECA, SERGEY V. LEVCHENKO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, 14195 Berlin, DE

The accurate description of transition-metal-containing defects in crystals presents a challenge for DFT with standard LDA and GGA functionals. Although replacing a fraction α of the (semi-)local exchange by the exact exchange (EX) in hybrid DFT reduces the self-interaction error, α remains a parameter depending on the target property. Here, the dependence of the formation energies of Fe_{Mg} substitutional defects in ferropericlase (Mg,FeO - the second most abundant mineral in Earth's lower mantle - on α in the Heyd-Scuseria-Ernzerhof hybrid functional (HSE) ($0 \leq \alpha \leq 1$, $\alpha = 0$ corresponds to PBE) is explored, and the results are compared to CCSD(T) embedded cluster calculations. We find that HSE($\alpha = 0.48$) reproduces the formation energy obtained with CCSD(T) and satisfies the constraint that the DFT HOMO equals the ionization energy as calculated by $G_0W_0@HSE(\alpha)$. Periodic models with converged unit-cell size are then used to calculate the atomic and electronic structure of Fe_{Mg} substitutional defect in MgO . The $O_h \rightarrow D_{4h}$ symmetry lowering (compressed FeO_6 octahedron) derived from experiments [1] is found for all α values (with HSE($\alpha = 0.25$) lattice parameter). However, the negative Δt_{2g} splitting of the Fe $3d$ states is obtained only for $\alpha \geq 0.4$. The calculated Δt_{2g} at these α values indicate a dynamic Jahn-Teller effect [1].

[1] T. Haupttricht et al., Phys. Rev. B 82, 035120 (2010).

15 min. coffee break

MM 62.5 Thu 17:00 H53

First-principles simulations of solid state NMR spectral parameters for metals with the GIPAW method — ●ARY FERREIRA, KARSTEN REUTER, and CHRISTOPH SCHEURER — Technische Universität München

Solid-state nuclear magnetic resonance (NMR) spectroscopy is a powerful tool for the characterization of a number of industry-relevant metallic materials like bulk metallic glasses or promising metallic anode materials in secondary lithium-ion batteries. For insulating solid materials, NMR chemical (or orbital) shifts can be successfully predicted from first-principles by all-electron density-functional theory calculations using localized basis sets in a cluster approach. Alternatively, the Gauge-Including Projector-Augmented Wave (GIPAW) method allows the use of periodic boundary conditions, plane waves and pseudopotentials. In both cases, the effect of the applied magnetic field on the electronic structure is simulated considering only the charge nature of electrons. However, for metals, the measured NMR shifts are dominated by their spin nature, resulting in the so-called Knight shifts. We address this limitation by implementing an extension of the GIPAW method to metals proposed in [1] within the framework of the open-source Quantum Espresso package. We report a set of preliminary computations of NMR spin and orbital shifts for bulk metallic Ag, Cu, and Cs, for which experimental reference values are available

in the literature. The encouraging results pave the way towards the application of the GIPAW method to real-world metallic systems. [1] Mayeul d'Avezac *et al.*, Phys. Rev. B **76**, 165122 (2007).

MM 62.6 Thu 17:15 H53

Efficient "On-the-Fly" Calculation of Raman Spectra from Ab-Initio Molecular Dynamics: Application to Lithium-Sulfur Batteries — ●POUYA PARTOVI-AZAR¹, THOMAS D. KÜHNE², and PAYAM KAGHAYCHI¹ — ¹Physical and Theoretical Chemistry, Freie Universität Berlin, Takustr. 3, D-14195 Berlin, Germany — ²Department of Chemistry, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

We present a novel computational method to accurately calculate Raman spectra from first principles. Together with an extension of the second-generation Car-Parrinello method to propagate maximally localized Wannier functions along with the nuclei, a speed-up of one order of magnitude can be obtained.

We have used this method to investigate the Raman spectra of $(\text{Li}_2\text{S}_4)_n$, $n = 1, 4, 8$ clusters which are believed to be the last intermediates in the $\text{S}_8 \rightarrow \text{Li}_2\text{S}$ transition in lithium-sulfur (Li-S) batteries during the discharge cycle. However, it is not fully established whether or not any other products coexist with the Li_2S crystal in the discharged state. In this study, we have observed a clear evidence of $\text{Li}_2\text{S}_4 \rightarrow \text{Li}_2\text{S}_2$ transition by investigating the systematic changes in the simulated Raman spectra as the cluster size increases. In line

with recent experiments, we found that the Raman-active sulfur-sulfur stretching mode at 440 cm^{-1} can be considered as a signature of covalent bonding between two and more sulfur atoms per formula. We have also demonstrated that the transition is mainly due to the strong electrostatic interactions between polar Li_2S_4 monomers.

MM 62.7 Thu 17:30 H53

Anisotropic magnetoresistance from the surface states of disordered topological insulators — ●HENRY LEGG and ACHIM ROSCH — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

In the presence of time-reversal symmetry electrons on the surface of a topological insulator cannot backscatter from disorder. A magnetic field parallel to the surface lifts this protection mechanism and enables backscattering which is predominantly in the direction parallel to the magnetic field. As a result the anisotropy of magnetoresistance parallel and perpendicular to \mathbf{B} is a sensitive probe of the loss of topological protection when time-reversal symmetry is broken.

Using a self-consistent T-matrix approximation we demonstrate how an in-plane magnetic field dramatically alters both the density of states and the resistivity of a topological insulator's surface. Our results are compared to experiments where the strong dependence on gate voltages provides an especially clear experimental signature of the scattering mechanism.

MM 63: Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Time: Friday 9:30–12:15

Location: H1

Invited Talk MM 63.1 Fri 9:30 H1
Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — ●ALLAN H MACDONALD — University of Texas at Austin, Austin TX, USA

The response of a conductor to a bias voltage is normally dominated by repopulation of states near the Fermi level. The transport steady state is fixed by a competition between acceleration in an electric field and disorder-induced scattering which attempts to restore equilibrium. This response of observables to a bias voltage is therefore extrinsic. There is however also response of states away from the Fermi level, which are polarized by the electric field. Provided that the typical band separation is larger than the finite life-time uncertainty in Bloch state energies this response is intrinsic, and for some observables it can be dominant. Intrinsic response coefficients are attractive targets for electronic structure theory because they are readily evaluated. Examples of responses to bias voltages that are sometimes dominantly intrinsic are the anomalous Hall conductivity of ferromagnetic or anti-ferromagnetic conductors, the spin-Hall conductivity of heavy metals, and current-induced torques in heavy-metal/ferromagnet systems. Intrinsic transport coefficients tend to be large in crystals with large momentum-space Berry curvatures, for example in crystals with topologically non-trivial electronic structure, and remain finite when a gap opens at the Fermi level to eliminate the Fermi surface. I will discuss some important examples of transport coefficients that are dominated by intrinsic contributions, mentioning as an important case the quantum anomalous Hall effect.

Invited Talk MM 63.2 Fri 10:00 H1
Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — ●JAIRO SINOVA — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

As current-driven torques are becoming more relevant in future MRAM technologies, in-plane current magnetization dynamics driven by the so called Rashba spin-orbit torques or through a combination of spin-Hall effect and spin-transfer torque has become more and more important. Understanding these torques is paramount to maximize their use. In recent experiments we have shown that in addition to the intrinsic SHE and STT effect there exists an intrinsic spin-orbit torque originating from the Berry phase of the spin-orbit coupled Bloch electrons analogous to the intrinsic spin Hall effect. This type of torques can be observed through SO-FMR driven experiments. We show this new type of torques in theory and experiments in GaMnAs and show that it can be of similar strength to the strong field-like torque. In

addition, we extend these physics to a new type of order-parameter manipulation by currents by examining the combined effect of spin-orbit coupling and anti-ferromagnetic order. We show that in broken inversion symmetry anti-ferromagnets a current will induce a non-equilibrium Néel-order field that will act directly on the Néel order parameter, hence making the direct manipulation of anti-ferromagnets without auxiliary exchange biased coupling to other ferromagnets a new and exciting possibility. One of these type of Néel torques has been recently experimentally confirmed.

Invited Talk MM 63.3 Fri 10:30 H1
Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — ●EWELINA HANKIEWICZ — Wuerzburg University

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band and the metallic gapless states at the edge [1]. Similarly, topological superconductors (TSC) have gapless zero energy states protected by the particle-hole symmetry, which in some cases form Majorana bound states. Here, we focus on the proximity-induced superconductivity in TIs [2] as well as on unusual properties of TSC [3] showing that they both can pave a road to find a Majorana state.

Concerning proximity-induced superconductivity in TIs, we describe a novel superconducting quantum spin-Hall effect, which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry even in magnetic fields [2]. We discuss unusual transport properties of this effect and possible Majorana detection schemes.

Finally, we discuss new systems like TSC on the hexagonal lattices. We develop combined microscopic and macroscopic description of these materials that predicts realistic scanning tunneling microscopy signal in these superconductors [3]. Is there a way to measure Majorana state in these systems?

[1] G. Tkachov and E. M. Hankiewicz, Review in Phys. Status Solidi B **250**, 215 (2013). [2] R. Reinthaler, G. Tkachov and E.M. Hankiewicz, Phys. Rev. B **92**, 161303(R) (2015). [3] L. Elster, C. Platt, R. Thomale, W. Hanke, and E. M. Hankiewicz, Nature Comm. **6**, 8232 (2015).

session break

Invited Talk MM 63.4 Fri 11:15 H1
Engineering Topological Quantum States: From 1D to 2D. — ●JELENA KLINOVAJA — University of Basel, Switzerland

I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered per demand. Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. I will discuss candidate materials such as semiconducting nanowires [1] and atomic magnetic chains [2]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [3,4]. Next, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [5-7], where interaction effects in the wires can be treated non-perturbatively via bosonization. Such systems can exhibit the integer or fractional quantum Hall effect, spin Hall effect, and anomalous Hall effect.

[1] J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012). [2] J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013). [3] J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014). [4] J. Klinovaja, A. Yacoby, and D. Loss, Phys. Rev. B 90, 155447 (2014). [5] J. Klinovaja and D. Loss, Phys. Rev. Lett. 111, 196401 (2013); J. Klinovaja and D. Loss, Eur. Phys. J. B 87, 171 (2014). [6] J. Klinovaja and Y. Tserkovnyak, Phys. Rev. B 90, 115426 (2014). [7] J. Klinovaja, Y. Tserkovnyak, and D. Loss, Phys. Rev. B 91, 085426 (2015).

Invited Talk

MM 63.5 Fri 11:45 H1

Skyrmions – Topological magnetization solitons for future spintronics — ●STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of chiral magnetic skyrmions – topological magnetization solitons – magnetic entities described by a micromagnetic energy functional with particle like properties that may open a new vista for spintronics. A crucial quantity for the chiral skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one- and two-dimensional lattices of chiral spin-textures, chiral domain walls and even single skyrmions. In retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give insight into the DMI, relating first-principles calculations to different models, discussing the transport properties of electrons *e.g.* the topological (THE) and anomalous (AHE) Hall effect in relation to the spin texture of a skyrmion, and discuss possibilities to tailor the magnetic interactions to enlarge the materials base to stabilize single skyrmions. – I acknowledge fruitful collaborations with D. Crum, J. Bouaziz, B. Dupé, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, A. Nandy, and B. Zimmermann.