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

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Overview of Invited Talks and Sessions

(Lecture rooms: H 0106, H 0107, TC 006, and TC 010; Posters: E)

Invited Talks

MM 2.1	Mon	9:30–10:00	TC 006	**Atomistic Mechanisms of Hydrogen Embrittlement** — •William Arthur Curtin
MM 12.1	Mon	15:00–15:30	TC 006	**Insights into phase transformations and microstructure development of TiAl alloys by use of advanced characterisation techniques** — •Florian Pyczak
MM 18.1	Tue	9:30–10:00	TC 006	**Unraveling the Mechanisms of Plasticity in Nanostructured Materials using Advanced Data Analysis and Simulation Methods** — •Alexander Stukowski
MM 29.1	Wed	9:30–10:00	TC 006	**The role of geometric boundaries on shape changes in biology** — •John Dunlop
MM 38.1	Wed	15:00–15:30	TC 006	**Spatiotemporal deformation dynamics in metals** — •Robert Maass
MM 43.1	Wed	18:30–19:00	TC 006	**Structural vs Chemical Adsorption Transitions at Surfaces & Interfaces** — •Wayne Kaplan
MM 44.1	Wed	19:00–19:30	TC 006	**Modelling solid-solid phase transformations: Atomistic insight on mechanisms and interface properties** — •Jutta Rogal
MM 47.1	Thu	9:30–10:00	TC 006	**Small experiments but great insights * Plasticity in brittle materials** — •Sandra Korte-Kerzel, Harshal Mathur, Sebastian Schröders

Invited talks of the joint symposium SYMM

See SYMM for the full program of the symposium.

SYMM 1.1	Thu	9:30–10:15	H 0105	**From MAX to MXene - From 3D to 2D** — •Michel Barsoum
SYMM 1.2	Thu	10:15–10:45	H 0105	**Structure evolution during low temperature growth of nanolaminate thin films** — •J.M. Schneider, L. Shang, H. Bolvardi, Y. Jiang, A. Al Gaban, D. Music, M. to Baben
SYMM 1.3	Thu	11:00–11:30	H 0105	**Autonomous healing of crack damage in MAX phase ceramics** — •Willem G. Sloof
SYMM 1.4	Thu	11:30–12:00	H 0105	**Magnetic MAX phases from first principles and thin film synthesis** — •Johanna Rosen
SYMM 1.5	Thu	12:00–12:30	H 0105	**Weak Field Magneto-Transport Properties of Mn+1AXn Phases** — •Thierry Ouisse, Lu Shi, Benoit Hackens, Benjamin Piot, Didier Chaussende

Invited talks of the joint symposium SYME

See SYME for the full program of the symposium.

SYME 1.1	Fri	9:30–10:00	H 0105	**Excitations and charge transfer phenomena in C based systems** — •Elisa Molinari
SYME 1.2	Fri	10:00–10:30	H 0105	**Towards optimal correlation factors for many-electron perturbation theories** — •Andreas Grüneis

SYME 1.3	Fri	10:30–11:00	H 0105	**Towards an ab-initio description of high temperature superconductivity** — •Garnet Chan
SYME 1.4	Fri	11:15–11:45	H 0105	**Correlation effects in unconventional superconductors: from micro- to nano- and macroscales.** — •Roser Valenti
SYME 1.5	Fri	11:45–12:15	H 0105	**Stochastic density functional and GW theories scaling linearly with system size** — •Roi Baer, Daniel Neuhauser, Eran Rabani

Sessions

MM 1.1–1.3	Sun	16:00–18:25	H 1058	**Tutorial: Electro Chemistry 4 Condensed Matter Physicists**
MM 2.1–2.1	Mon	9:30–10:00	TC 006	**Invited talk Curtin**
MM 3.1–3.5	Mon	10:15–11:45	H 0106	**Microstructure and Phase Transformations**
MM 4.1–4.5	Mon	10:15–11:45	H 0107	**Liquid and Amorphous Metals I: Fragility and Dynamics of Metallic Glasses**
MM 5.1–5.4	Mon	10:15–11:45	TC 006	**Hydrogen in Metals: Ab initio approaches**
MM 6.1–6.5	Mon	10:15–11:45	TC 010	**Functional Materials I: Battery Materials**
MM 7.1–7.5	Mon	11:45–13:00	H 0106	**Microstructure and Phase Transformations II**
MM 8.1–8.5	Mon	11:45–13:00	H 0107	**Liquid and Amorphous Metals II: Structure Formation in Metallic Glasses**
MM 9.1–9.5	Mon	11:45–13:15	TC 006	**Hydrogen in metals II: Multiscale simulations**
MM 10.1–10.5	Mon	11:45–13:00	TC 010	**Functional materials II: Battery Materials**
MM 11.1–11.10	Mon	14:30–17:15	EB 202	**Biomaterials and Biopolymers I (joint BP/CPP)**
MM 12.1–12.1	Mon	15:00–15:30	TC 006	**Invited talk Pyczak**
MM 13.1–13.4	Mon	15:45–16:45	H 0106	**Microstructure and Phase Transformations III**
MM 14.1–14.7	Mon	15:45–17:45	H 0107	**Transport I: Diffusion**
MM 15.1–15.7	Mon	15:45–18:00	TC 006	**Hydrogen in metals III: Experiments**
MM 16.1–16.7	Mon	15:45–17:45	TC 010	**Functional materials III: Sensors and Actuators**
MM 17.1–17.34	Mon	18:00–20:00	Poster E	**Postersession I**
MM 18.1–18.1	Tue	9:30–10:00	TC 006	**Invited talk Stukowski**
MM 19.1–19.5	Tue	10:15–11:45	H 0106	**Methods in Computational Materials Modelling I: Materials Design**
MM 20.1–20.5	Tue	10:15–11:30	H 0107	**Liquid and Amorphous Metals III: Deformation of Metallic Glasses**
MM 21.1–21.4	Tue	10:15–11:45	TC 006	**Hydrogen in metals IV: Special topics**
MM 22.1–22.5	Tue	10:15–11:45	TC 010	**Functional Materials IV: Thermoelectric and Multiferroic Materials**
MM 23.1–23.4	Tue	11:45–12:45	H 0106	**Methods in Computational Materials Modelling: Battery Mateirals**
MM 24.1–24.4	Tue	11:45–12:45	H 0107	**Transport II: Thermal and Electrical Conductivity**
MM 25.1–25.5	Tue	11:45–13:15	TC 006	**Hydrogen in Metals V: H in Steels**
MM 26.1–26.5	Tue	11:45–13:00	TC 010	**Functional Materials V: Functional Materials**
MM 27.1–27.7	Tue	14:00–15:45	A 053	**Transport: Nanomechanics (joint session with MM)**
MM 28.1–28.35	Tue	18:30–20:30	Poster E	**Poster Session II**
MM 29.1–29.1	Wed	9:30–10:00	TC 006	**Invited talk Dunlop**
MM 30.1–30.5	Wed	10:15–11:45	H 0106	**Methods in Computational Materials Modelling III: Thermodynamics**
MM 31.1–31.5	Wed	10:15–11:30	H 0107	**Liquid and Amorphous Metals IV: Structure and Electronic Properties of Glasses**
MM 32.1–32.3	Wed	10:15–11:45	TC 006	**Biomaterials and Biological materials I**
MM 33.1–33.4	Wed	10:15–11:30	TC 010	**Structural Materials I: Phase Stability and Mechanical Properties**
MM 34.1–34.3	Wed	11:30–12:15	TC 010	**Structural Materials II: Brazing and Welding**
MM 35.1–35.6	Wed	11:45–13:15	H 0106	**Methods in Computational Materials Modelling IV: Steels**
MM 36.1–36.4	Wed	11:45–12:45	H 0107	**Nanomaterials I: Excess Volume and Confinement**
MM 37.1–37.5	Wed	11:45–13:15	TC 006	**Biomaterials and Biological Materials II**
MM 38.1–38.1	Wed	15:00–15:30	TC 006	**Invited talk Maass**
MM 39.1–39.7	Wed	15:45–17:45	H 0106	**Methods in Computational Materials Modelling V: Kinetics and Beyond DFT**
MM 40.1–40.8	Wed	15:45–18:00	H 0107	**Nanomaterials II: Mechanical Properties**
MM 41.1–41.6	Wed	15:45–17:15	TC 006	**Electron Microscopy**

MM 42.1–42.8	Wed	15:45–18:00	TC 010	**Mechanical Properties I**
MM 43.1–43.1	Wed	18:30–19:00	TC 006	**Invited talk Kaplan**
MM 44.1–44.1	Wed	19:00–19:30	TC 006	**Invited talk Rogal**
MM 45	Wed	20:00–21:00	TC 006	**General Meeting of the Metal- and Materials Physics Division and Presentation of the Best Poster Award**
MM 46.1–46.8	Thu	9:30–13:00	EB 407	**Focused Session on GHz Dielectrics: Materials for Mobile Communication I (jointly with HL, MM, DY)**
MM 47.1–47.1	Thu	9:30–10:00	TC 006	**Invited talk Korte**
MM 48.1–48.5	Thu	10:15–11:30	H 0106	**Methods in Computational Materials Modelling VI: Algorithms**
MM 49.1–49.5	Thu	10:15–11:45	H 0107	**Interfaces I: Structure and Segregation**
MM 50.1–50.3	Thu	10:15–11:45	TC 006	**Biomaterials and Biological Materials III**
MM 51.1–51.5	Thu	10:15–11:45	TC 010	**Mechanical properties II**
MM 52.1–52.6	Thu	11:45–13:15	H 0106	**Nanomaterials III: Nanoporous Gold and Phase Transformations**
MM 53.1–53.3	Thu	11:45–12:30	H 0107	**Interfaces II: Deformation and Motion**
MM 54.1–54.5	Thu	11:45–13:00	TC 006	**Biomaterials and Biological Materials IV**
MM 55.1–55.4	Thu	11:45–12:45	TC 010	**Mechanical Properties III**
MM 56.1–56.5	Thu	15:00–17:00	EB 407	**Focused Session on GHz Dielectrics: Materials for Mobile Communication II (jointly with HL, MM, DY)**
MM 57.1–57.5	Fri	9:30–12:15	H 0105	**Frontiers of Electronic Structure Theory: Many-body Effects on the Nano-scale**

Annual General Meeting of the Metal and Material Physics Division and Best Poster Award

Mittwoch 20:00–21:00 TC 006

- Bericht
- Wahl
- Verschiedenes

MM 1: Tutorial: Electro Chemistry 4 Condensed Matter Physicists

Organized by Erich Runge and Jörg Neugebauer on behalf of the Semiconductor Physics Division (HL) and the Metal and Material Physics Division (MM), respectively.

Time: Sunday 16:00–18:25 Location: H 1058

Invited Talk MM 1.1 Sun 16:00 H 1058

Challenges in the theoretical description of structures and processes at electrochemical interfaces — •Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — Helmholtz Institut Ulm, 89069 Ulm, Germany

In spite of its technological relevance in the energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces is still rather limited. The theoretical description of these interfaces is hampered by three challenges [1]. i) In electrochemistry, structures and properties of the electrode-electrolyte interfaces are governed by the electrode potential which adds considerable complexity to the theoretical treatment since charged surfaces have to be considered. ii) The theoretical treatment of processes at solid-liquid interfaces includes a proper description of the liquid which requires to determine free energies instead of just total energies. This means that computationally expensive statistical averages have to be performed. iii) Electronic structure methods based on density functional theory (DFT) combine numerical efficiency with a satisfactory accuracy which makes them appropriate for electrochemical systems. However, there are severe shortcomings of the DFT description of liquids, in particular water, using current functionals.

In this tutorial talk, I will give an overview over concepts and theoretical methods for the realistic description of electrochemical interfaces. Examples of insights gained from theoretical studies will be presented but open challenges will be identified as well.

[1] N.G. Hörmann *et al.*, J. Power Sources **275**, 531 (2015).

Short break

Invited Talk MM 1.2 Sun 16:50 H 1058

Raman under water - Of photons, phonons and the fun of tuning the Fermi level — •Katrin F. Domke — MPI for Polymer Research, Ackermannweg 10, D-55128 Mainz

t.b.a.

Short break

Invited Talk MM 1.3 Sun 17:40 H 1058

Scanning probe microscopies for electrochemical problems — •Gunther Wittstock — Carl v. Ossietzky University of Oldenburg, School of Mathematics and Science, Department of Chemistry, D-26111 Oldenburg

Electrified solid-liquid interfaces are characterized by a vertical and horizontal inhomogeneity in structure. Even well prepared single crystal electrodes show, adatoms, steps kinks and other defects. The investigation of such structures by STM has dramatically enhanced our understanding of such interfacial structures. However, the experiments were mostly performed in the absence of a Faradayic reaction (.i.e. electrolysis). With a few exceptions, electrodes are designed for controlling Faradayic reactions. High current densities are requested for efficient energy conversion devices; very low current densities are a requirement for materials that shall resist corrosion under harsh environments. Such materials (polycrystalline, multiphase or composites) show a large variation of local current densities that are neither accessible by I-V-curves nor by STM. Scanning electrochemical microscopy (SECM) provides this information. It uses the electrolysis current of a dissolved redox-active compound at a probe microelectrode to generate the signal. The electrolysis at the probe is coupled to local reaction at the sample by diffusion of reactants in the probe-sample gap. Different working modes and examples will be explained with the aim to differentiate between fundamental barriers and current instrumental limitations that might be overcome by the impact of well trained physicist.

MM 2: Invited talk Curtin

Time: Monday 9:30–10:00 Location: TC 006

Invited Talk MM 2.1 Mon 9:30 TC 006

Atomistic Mechanisms of Hydrogen Embrittlement — •William Arthur Curtin — EPFL, Lausanne, Switzerland

A number of concepts, such as Hydrogen Enhanced Localized Plasticity and Hydrogen Enhanced Decohesion, have been proposed to explain Hydrogen embrittlement in different metallic systems. Here, we first present atomistic models some of proposed mechanisms and find limited evidence for their operation. We then discuss a new mechanism wherein H accumulates at nanometer scales around any pre-existing crack tip, which shuts off the crack tip dislocation emission and thereby eliminates crack blunting, suppresses ductile failure modes, and fracture occurs by cleavage through the brittle H-rich region. The process is self-sustaining through continual H transport to the crack tip region. We demonstrate operation of this mechanism in Fe-H using direct atomistic simulations. We then connect the nanoscale mechanism to experimental conditions via the kinetics of H diffusion to the crack tip region, and predict embrittlement as a function of loading rate, H chemical potential, temperature, and H diffusion rate. Application of new model leads to predictions of embrittlement across a range of typical Fe-based systems that are in very good agreement with experimental results.

MM 3: Microstructure and Phase Transformations

Time: Monday 10:15–11:45 Location: H 0106

MM 3.1 Mon 10:15 H 0106

Phase field simulations of grain boundary wetting and melting kinetics — •Venkata Sai Pavan Kumar Bhogireddy[1], Claas Hüter[1], Jörg Neugebauer[1], Oleg Shchyglo[2], Ingo Steinbach[2], and Robert Spatschek[1] — [1]Max Planck Institute for Iron Research, Düsseldorf, Germany — [2]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-University Bochum, Bochum, Germany

Grain boundary premelting is known as the phenomenon that a thin melt layer can appear between two grains already below the bulk melting point, which can cause material failure. It results from a short-ranged structural interaction between the nearby solid-melt interfaces, which are induced by the overlap of the crystal structures in the sandwiched melt. The classical prediction for the transition between wetting and non-wetting states at the melting point is $2\sigma_{sl} = \sigma_{gb}$, where σ_{sl} is the solid-melt interface energy and σ_{gb} the dry grain boundary energy. Here we report on theoretical and numerical investigations of this phenomenon using a multi-order parameter phase field model based on obstacle potentials. We find that the premelting transition is in agreement with the classical expectation, and the short-ranged interactions are predicted.

Beyond this static perspective we report on the kinetics of grain boundary melting along dry and overheated low angle grain boundaries. A steady state regime for the diffusion limited growth is found in the phase field simulations, and the melting velocity depends on the aforementioned short-ranged structural interactions. The velocities are qualitatively in agreement with a sharp interface theory.

MM 3.2 Mon 10:30 H 0106

Influence of short-range forces on melting along grain boundaries — •Claas Hüter[1], Fabian Twiste[1], Efim A. Brener[2], Jörg Neugebauer[1], and Robert Spatschek[1] — [1]Computational Materials Design Department, Max-Planck Institut für Eisenforschung, Düsseldorf, Germany — [2]Peter-Grünberg-Institut 2, Forschungszentrum Jülich, Jülich, Germany

In metallurgical processing, elevated temperatures and reduced local transition temperatures can lead to phenomena of grain boundary induced failure, as e.g. hot cracking. We introduce a model which couples diffusional melting and nanoscale structural forces in a combined nano-mesoscale sharp-interface description. We obtain analytic and numerical solutions for melting processes at grain boundaries influenced by structural disjoining forces, focusing on the experimentally relevant regime of small deviations from the melting temperature. Though spatially limited to the close vicinity of the tip of the propagating melt finger, the influence of the disjoining forces yields a strong modification of the penetration velocity. Close to equilibrium the atomistic effects near the triple junctions can be expressed through a contact angle renormalization in a mesoscale formulation. For higher driving forces, significantly higher melting velocity than predicted from a purely mesoscopic description are found.

MM 3.3 Mon 10:45 H 0106

Ab initio interpretation of the abnormal carbon redistribution during martensitic transformation in Fe-C alloys — •Xie Zhang[1,2], Tilmann Hickel[1], Jutta Rogal[2], Ralf Drautz[2], and Joerg Neugebauer[1] — [1]Max-Planck-Insitut für Eisenforschung GmbH, Düesseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, Bochum, Germany

As a key feature of the martensitic transformation in Fe-C alloys, the abnormally low tetragonality resulting from the C redistribution is a historically pending problem. To address this issue, we developed an atomistic model for the martensitic transformation in Fe-C alloys and calculated the corresponding minimum energy paths with ab initio nudged elastic band simulations. Our insights provide a theoretical evidence for the C redistribution into different octahedral sublattices in martensite, and thus nicely explain the occurrence of the abnormally low tetragonality. It also allows us to interpret the mechanism for the martensitic transition as a combination of a tetragonal cell deformation and atomic shuffling and thus our understanding of the microstructure evolution in steels.

MM 3.4 Mon 11:00 H 0106

Atomistic simulation of the martensitic phase transition in the iron-nickel system — •Emilia Sak-Saracino and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS,Erwin-Schrödinger-Straße, 67663 Kaiserslautern, Germany

Nickel is one of the most important alloying elements in steel manufacture because of its slow rate of oxidation at room temperature and also as a material for ultra-high-strength steels where the strength does not originate from carbon interstitials, but from inter-metallic compounds. By using molecular dynamics simulation, we investigate the behavior of the martensitic phase transition in the iron-nickel system. We observe this transition by imposing a heating/cooling cycle on the system and monitoring the hysteresis of the system volume with temperature. In addition we report the change of the lattice constant and of the average cohesive energy as a function of nickel content.

MM 3.5 Mon 11:15 H 0106

Localizing sources of acoustic emission during the martensitic transformation — •Robert Niemann[1,2], Jaromír Kopeček[3], Oleg Heczko[3], Jan Romberg[1], Ludwig Schultz[1,2], Sebastian Fähler[1,2], Eduard Vives[4], Lluís Mañosa[4], and Antoni Planes[4] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — [3]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 02 Prague, Czech Republic — [4]Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona. Diagonal 647, 08028 Barcelona, Catalonia, Spain

Acoustic avalanches are a feature of solids under stress e.g arising from martensitic phase transitions. Local sources of acoustic emission are studied in order to enlight the microscopic mechanisms. From two-dimensionally resolved acoustic emission measurement and simultaneous optical observation of the surface we identify microstructural events at the phase boundary that lead to acoustic emission [1]. A resolution in the 0.1 mm-range was reached for the location of acoustic emission sources on a Ni-Mn-Ga polycrystal. The acoustic activity and the size distribution of the microstructural transformation events exhibit power-law behavior. The origin of the acoustic emission are elastically incompatible areas, such as differently oriented martensitic plates and grain boundaries in proximity to transforming grains. We propose a model to explain the decrease of the critical exponent in mechanical or magnetic fields. [1] Phys. Rev. B. 89, 214118 (2014)

15 min. break

MM 4: Liquid and Amorphous Metals I: Fragility and Dynamics of Metallic Glasses

Time: Monday 10:15–11:45 Location: H 0107

MM 4.1 Mon 10:15 H 0107

Thermodynamic Properties of Zr- and Au-based Bulk Metallic Glasses at Very Low Temperatures — •Andreas Reifenberger, Daniel Rothfuss, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

Many low temperature properties of glasses can be described by the standard tunnelling model. Dielectric glasses and metallic glasses in the superconducting state far below T_c ought to yield similar results since their behaviour is dominated by interactions between tunnelling systems and phonons as electrons condense to cooper pairs. We present measurements of the specific heat and thermal conductivity of superconducting bulk metallic glasses (based on Zr and Au, respectively) in the temperature range from 6 mK to 1 K. We discuss these measurements in the framework of both the BCS-theory of superconductivity and the standard tunnelling model. In the superconducting state close to T_c, where interactions with quasi-particles need to be taken into account, both measurements agree well with BCS-theory predictions. Far below T_c we find good agreements between our data and the standard tunnelling model predictions.

MM 4.2 Mon 10:30 H 0107

Time Dependent Nonlinear Response in Glassy Systems — •Birte Riechers[1], Ranko Richert[2], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Department of Chemistry & Biochemistry, Arizona State University, USA

Relaxation modes, especially their detailed description and understanding, play a major role for scientists working with glassy matter. One of many interesting aspects is the time scale of the change in fictive temperature under harmonic excitation in the nonlinear response regime[a].

By applying an external force sufficiently high to achieve nonlinear response, relaxation modes are excited. A time resolved measurement of the energy loss in glassy materials during a jump from the linear to the nonlinear response regime reveals the time scale of energy redistribution within the relaxation spectrum.

The behavior of plastic crystals, and metallic glasses was investigated experimentally using dielectric spectroscopy (DES), and dynamic mechanical analysis (DMA), respectively. Results are discussed with a focus on the behavior of fictive temperature regarding a connection to structural relaxation.

Financial support by the DFG Research Unit FOR 1394 is acknowledged.

[a] R.Richert, J.Chem.Phys. 130, 194509, 2009

MM 4.3 Mon 10:45 H 0107

Atomic dynamics in Zr-based glass forming melts — Sri Wayuni Basuki[1], Elisabeth Gill[1], Klaus Rätzke[1], •Franz Faupel[1], Fan Yang[2], and Andreas Meyer[2] — [1]Univ. Kiel, Chair for Multicomponent Materials, D-24143 Kiel, Germany — [2]DLR, D-51170 Köln, Germany

Recently, we reported a strong decoupling of Zr-95 and Co-57 radiotracer diffusivities in a bulk metallic glass forming $Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$ melt (Vitreloy 4) far above the liquidus temperature [1] suggesting the development of solid-like, i.e. energy-landscape controlled, features already in the stable liquid state more than 300 K above the mode coupling T_c [1]. Meanwhile, we performed similar simultaneous radiotracer diffusion experiment of Co-57 and of Zr-95 in binary Zr-Ni and ternary Zr-Ni-Al alloys with a largely reduced glass-forming ability above the liquidus temperature. Here, a much less pronounced decoupling was observed. The results will be discussed in terms of recent theoretical approaches on atomic dynamics of metallic melts.

[1] S. W. Basuki, A. Bartsch, F. Yang, K. Rätzke, A. Meyer, and F. Faupel, Phys. Rev. Lett. 113, (2014) 165901

MM 4.4 Mon 11:00 H 0107

Interatomic Repulsion Controls the Fragility of Supercooled Metallic Melts — •Johannes Krausser and Alessio Zaccone — Department of Physics, Technische Universität München, 85748 Garching, Germany

We present an analytic scheme to connect the fragility and glass-forming properties of metallic glasses to the pseudopotential between ionic cores in the metal. This is achieved by a suitable approximation of the repulsive part of the interaction and by using non-affine lattice dynamics to obtain analytical expressions for the shear modulus, viscosity, and fragility in terms of the pseudopotential. Employing a one-parameter fit to experimental data for various alloys, we were able to link the steepness of the interionic repulsion to the Thomas-Fermi-screened Coulomb repulsion and to the Born-Mayer valence electron overlap repulsion (due to Pauli exclusion). This leads, for the first time, to a simple closed-form expression for the fragility of the supercooled liquid metal in terms of atomic-scale interaction parameters. In particular, a relationship of linear proportionality is found between the fragility and the energy scales of both the screened Coulomb repulsion and the valence electron repulsion due to Pauli exclusion. The new fundamental law that we discovered opens up opportunities to fabricate alloys with tailored thermo-elastic and glass-forming properties by tuning the interatomic interaction parameters via the electronic structure and chemical composition of the alloy.

MM 4.5 Mon 11:15 H 0107

Fictive temperature and glass transition temperature of a metallic glass investigated by fast scanning calorimetry — •Christian Simon, Joachim Bokeloh, Jonas Bünz, and Gerhard Wilde — Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48155 Münster

The use of fast scanning calorimeters allows a new access to thermal analysis experiments on metallic glasses. The glass transition and the crystallization were often in the focus of different studies. These studies are often limited by the heating and cooling rates of the conventional devices. The fast scanning calorimeters allow the investigation of glass transition and crystallization at high rates. The fictive temperature of glass is the temperature at which the structure of an equilibrium liquid is frozen-in. The determination of the fictive temperature is usually done by a heat capacity matching method. The strong requirement of a defined thermal history is often a difficult task for the determination of fictive temperature in the case of metallic glasses. The fast scanning calorimeter allows the in-situ production of metallic glasses and thus leads to a reproducable thermal history of the sample for every single measurement. We present data from a AuSi based metallic glass investigated by a fast scanning calorimter (50 K/s - 20 000 K/s). The obtained data cover a wide kinetic regime and are discussed with respect of deviations from Arrhenius behavior at higher heating rates.

15 min. break

MM 5: Hydrogen in Metals: Ab initio approaches

Time: Monday 10:15–11:45 Location: TC 006

Topical Talk MM 5.1 Mon 10:15 TC 006

Atomistic simulations of microstructural defects and their role in H trapping and diffusion — •Matous Mrovec[1], Davide Di Stefano[1], Christian Elsässer[1], Roman Nazarov[2], and Tilmann Hickel[2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — [2]Max-Planck Institute for Iron Research, Düsseldorf, Germany

A correct description of hydrogen diffusion and trapping is prerequisite for understanding the phenomenon of hydrogen embrittlement. The macroscopic H diffusion in bulk materials has been studied extensively in the past both experimentally and theoretically. Nevertheless, the knowledge of microscopic diffusion processes, especially in distorted environments around crystal defects, is still limited. In this study we apply atomistic simulations to investigate the diffusion and trapping of hydrogen in Fe and Ni using accurate first-principles methods based on the density functional theory. Our results show that the diffusion barriers can indeed vary significantly in the vicinity of crystal defects, imperfections and interfaces. The calculations also confirm that a proper treatment of quantum effects is crucial for a reliable theoretical description of H diffusion, in particular for bcc Fe. Several examples of H trapping at grain and phase boundaries will be presented and analyzed.

MM 5.2 Mon 10:45 TC 006

Hydrogen at the ferrite-cementite and ferrite-austenite interfaces — •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, Germany

In the present contribution, detailed simulations of the hydrogen behaviour in the vicinity of the ferrite-cementite and ferrite-austenite interfaces have been performed. The effects of hydrogen trapping and diffusion, as well as the interaction of hydrogen with vacancies near the interface, have been studied. To elucidate more clearly the effect of hydrogen on the mechanical properties of the interfaces, a series of simulated tensile tests have been performed, which shed light on specific mechanisms of the hydrogen embrittlement effect.

The results of such simulations can also be used as benchmarks for large-scale atomistic simulations, in particular for the development of potentials based on the tight-binding approximation, so that hydrogen behaviour in the vicinity of extended defects, such as nanovoids and dislocations, can be simulated. The generation of such a model, and initial test calculations based upon it, will be demonstrated.

MM 5.3 Mon 11:00 TC 006

Hydrogen trapping at vacancies and hydrogen impact on vacancy diffusion and self-diffusion in Ni. — Yu Wang[1,2], Damien Connétable[2], and •Döme Tanguy[1] — [1]Institut Lumière Matière, UMR 5306, Université Lyon 1-CNRS, Villeurbanne, France — [2]CIRIMAT,UMR 5085, ENSIACET, Toulouse, France

We have performed EAM and DFT calculations of H segregation energies at vacancies in Ni. The maximum binding is 0.27eV and 0.4eV in the single and divacancy respectively, in good agreement with Fukai's Thermal Desorption Spectroscopy results. By a comprehensive calculation of the formation energy of VHn clusters (n=1 to 14), it was shown that segregation occurs mostly on the octahedral site (off-centered) in the vacancy (O1) with almost no O1-O1 interactions, strong O1-T1 (tetrahedral) repulsion and weak attractive O1-O2 interaction. Approximately constant effective pair interactions can be extracted from these formation energies. Together with the segregation energies in the dilute limit, they constitute a simple energetic model from which we can derive the equilibrium distributions and concentrations of VHn (analytical formulas are validated against Monte Carlo simulations). A good separation of timescales between H diffusion events and vacancy-metal exchanges enables a simple calculation of the diffusion coefficient of the clusters from the equilibium distribution and a limited set of barriers. H drastically slows down the vacancies, but this effect is overcompensated by the increase in equilibrium vacancies and finally Ni self-diffusion is markedly increased.

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MM 5.4 Mon 11:15 TC 006

Hydrogen embrittlement of a carbon segregated symmetrical tilt grain boundary in α-Fe — Arshad Tahir, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, 44780 Bochum

The cleavage strength of a symmetrical tilt grain boundary (STGB) in body centred cubic (bcc) Fe is investigated by means of ab-initio calculations with respect to the effect of a varying number of C and H atoms at the grain boundary. Our results indicate that hydrogen enhanced decohesion of interfaces in Fe-C alloys could be understood as a co-segregation effect.
The calculated segregation energy for C shows that in a bcc Fe-C system with a sufficient amount of interstitial C, the C segregated state should be considered as the ground state of this interface. The work of separation as well as the tensile strength increase significantly with increasing C content. A partial exchange of C with hydrogen changes the cohesion enhancing elastic contribution of C to an embrittling contribution, and also reduces the beneficial chemical contribution to the cohesion. The reduction in strength amounts to almost 20% in the co-segregated case, and to more than 25% if C is completely replaced by H. Compared to the strength of the STGB in pure iron, however, the influence of H is negligible. Hence, H embrittlement of this interface can only be understood in the three component Fe-C-H system.

15 min. break

MM 6: Functional Materials I: Battery Materials

Time: Monday 10:15–11:45 Location: TC 010

MM 6.1 Mon 10:15 TC 010

Ultra-Thin All Solid-State Thin-Film Batteries — •Susann Nowak[1], Frank Berkemeier[2], and Guido Schmitz[1] — [1]Lehrstuhl für Materialphysik, Universität Stuttgart — [2]Institut für Materialphysik, Universität Münster

This talk focuses on ultra-thin all solid-state batteries with an overall thickness below 1 μm. They are prepared with a very good layer quality (roughness below 5 nm) via ion beam sputtering. The homogeneity and structure of the layers and interfaces is proven by cross-section TEM. The studied all solid-state batteries are composed of lithium iron phosphate as a cathode (LFP), lithium phosphorous oxynitride (LiPON) as an electrolyte and Sn or Si as an anode. Battery cells can be charged and discharged more than 100 cycles, still showing more than 50% of the initial capacity. The observed cycling behavior is strongly temperature dependent, exhibiting a increase of the capacity with elevated temperatures. The observed potential curve is compared to the expected one taking into account the charge-discharge behavior of the single electrodes. The influences of the balancing of the electrodes and the lithiation state of the anode on the energy density as well as the observed cell potentials are also discussed.

MM 6.2 Mon 10:30 TC 010

Electrically-induced interface reactions in lithium ion batteries — •Frank Berkemeier and Fabian Inkmann — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

An unconventional type of thin film lithium ion battery will be presented, which consists of a lithium phosphorous oxynitride (LiPON) thin film that is embedded between a silver and a platinum layer. All layers are prepared by sputter deposition, resulting in a triple layer stack of a thickness well below 1 μm.

We demonstrate that it is possible to trigger an electrochemical reaction between LiPON and silver, when applying a negative voltage of about -3.8 V to the silver electrode. This interface reaction causes

the growth of an interface reaction layer, which is capable to reversibly intercalate/deintercalate lithium.

To understand the properties of this layer in more detail, the structural and electrochemical properties of the overall layer stacks before and after electrochemical treatment have been investigated by e.g. impedance spectroscopy, cyclic voltammetry, and transmission electron microscopy. In course of these experiments it has been found that the cells exhibit a well-defined charge/discharge behavior and a promising cycling stability. Moreover, detailed informations about the morphology of the reaction layer have been obtained, as well as data about its growth kinetics and its lithium storage capacity.

MM 6.3 Mon 10:45 TC 010

Self-forming Lithium Ion Batteries: Optimization of Ag-LiPON Devices — •Leila Raafat, Susann Nowak, and Guido Schmitz — Chair of Materials Physics, University of Stuttgart

Sandwiching the solid electrolyte lithium phosphorous oxynitride (LiPON) between two current collectors leads to a thin-film battery after initial charging (Liu et al., J. Electrochem. Soc. 155 (1), A8 (2008)). These electrochemically formed batteries are of particular interest, since the Li anode is internally electroplated without concern of its contamination. Three different devices of this design with a thickness of ca. 1μm were electrochemically investigated. We discovered that employing an inert anode current collector towards LiPON like copper (Cu), will lead to Cu/LiPON/Ag-devices which can withstand over 500 cycles showing a stable discharge capacity. Since dendrite formation at the interfaces of such a device is inevitable, short circuits can occur. Extending a concept reported by Yourey et al. (Electrochim. Acta 66, 193 (2012)), the formation of short circuits can be prevented by using a Li oxide based solid electrolyte interphase between the Li anode and LiPON. Therefore, we modified the devices by depositing a thin layer of lithium phosphate on the Cu current collector. This adjustment resulted in a significantly increased success rate and an improved cycle life; over 2000 cycles were measured. In order to understand the reactions happening within these batteries, the kinetics of the reaction layer are investigated depending on the cycle number.

MM 6.4 Mon 11:00 TC 010

$LiCoO_2$ and $LiFePO_4$ thin-films for application in lithium ion batteries — •Martin Fiedler[1], Antonia Reyes Jimenez[2], Frank Berkemeier[1], and Guido Schmitz[3] — [1]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Universität Münster, MEET - Batterieforschungszentrum, Corrensstr. 46, 48149 Münster — [3]Universität Stuttgart, Institut für Materialwissenschaft, Heisenbergstraße 3, 70569 Stuttgart

In commercial lithium ion batteries, powders of Lithium Cobalt Oxide (LCO) or Lithium Iron Phosphate (LFP) are commonly used as cathode materials. Contrary to this common approach, in this work LCO and LFP electrodes are prepared by magnetron sputtering, resulting in films of a thickness between 120 and 5500 nm. After deposition, the layers are characterized by X-ray diffraction, electron microscopy, and different electrochemical techniques. In particular, the influence of post annealing and in situ heating of the films in a temperature range between 400 and 700°C is investigated, and it is found that the electrochemical performance of the layers significantly depends on both parameters. Moreover, it is demonstrated that, despite their large thickness, the cathodes are mechanically stable during cyclic lithiation/delithiation and thus allow detailed investigations of transport kinetics without being influenced by varying interface effects. In course of these measurements, the diffusion of lithium is investigated by means of electrochemical techniques, and is correlated to the microstructure of the layers. Finally, the technical relevance of the sputtered layers in functional full cells is presented.

MM 6.5 Mon 11:15 TC 010

Charging-induced defects in $Li_{1-x}CoO_2$ battery electrodes — •Gregor Klinser[1], Stefan Topolovec[1], Peter Parz[1,4], Heinz Krenn[2], Harald Kren[3], Stefan Koller[3], and Roland Würschum[1] — [1]Institute of Materials Physics, Graz University of Technology, Austria — [2]Institute of Physics, University of Graz, Austria — [3]VARTA Micro Innovation GmbH, Graz, Austria — [4]now at: Magna Steyr Battery Systems GmbH & Co OG, Zettling, Austria

Research in the field of modern battery materials demands characterization techniques which allow an inspection of atomistic processes during battery charging and discharging. In the present work, SQUID magnetometry is combined with positron annihilation spectroscopy to study the battery cathode material $Li_{1-x}CoO_2$ in dependence of the degree of charging.
Positron annihilation measurements reveal vacancy-type defects on the Li-sublattice the size of which increases with Li-extraction [1]. The concomitant increase of the magnetic moment with Li-extraction by SQUID magnetometry cannot exclusively be attributed to $Co^{3+} \rightarrow Co^{4+}$ oxidation, however, may also involve oxygen states. In the vicinity of the reversibility limit of charging, a sharp drop of the localized magnetic moment is observed, which may be linked to the Li vacancy reordering recorded by positron annihilation spectroscopy [1].

[1] P. Parz, B. Fuchsbichler, S. Koller, B. Bitschnau, F. Mautner, W. Puff and R. Würschum, Appl. Phys. Lett. 102, 151901 (2013).

15. min break

MM 7: Microstructure and Phase Transformations II

Time: Monday 11:45–13:00 Location: H 0106

MM 7.1 Mon 11:45 H 0106

Shake, rattle and roll! Direct measurement of grain rotations during Ostwald ripening in semisolid Al-5 wt% Cu — Jules Dake[1], Jette Oddershede[2], Thomas Werz[1], Henning Osholm Sørensen[3], Søren Schmidt[2], and •Carl Emil Krill III[1] — [1]Ulm University, Germany — [2]Technical University of Denmark, Denmark — [3]University of Copenhagen, Denmark

Materials scientists studying the coarsening of crystalline solids have long speculated that individual crystallites can undergo rigid-body rotation while shrinking or growing by the usual mechanism of boundary migration. The driving force for such grain rotations would be a reduction in interfacial energy: if two grains rotate toward each other's orientation, the boundary between them will become smaller in angle or even vanish, thereby lowering the free energy of the system. Investigations of spherical grains placed on single-crystalline substrates have lent credibility to this hypothesis; however, it remains to be determined whether grain rotation also takes place under technically relevant conditions, such as the sintering of closely packed powders or the Ostwald ripening of a two-phase material. Employing the recently developed technique of three-dimensional x-ray diffraction (3DXRD) microscopy, we have obtained direct evidence for the occurrence of grain rotations in a bulk, semisolid Al-Cu alloy undergoing Ostwald ripening. Not only did we find that the magnitude of grain rotations increases with relative volume of the liquid phase (as one might naively expect), but we also discovered that the orientation dependence of the interfacial energy biases the direction of rotation.

MM 7.2 Mon 12:00 H 0106

Anomalous Grain Growth in Friction Stir Welded Aluminium — •Michael Kreissle[1], Janina Diessenbacher[1], Sahin Sünger[2], and Ferdinand Haider[1] — [1]Univ. Augsburg, Inst. f. Physik, 86135 Augsburg — [2]TU München, Inst. f. Werkzeugmaschinen und Betriebswissenschaften, 85748 Garching

Friction Stir Welding is a solid state joining technique using a rotating, forward moving tool, which plastifies and locally mixes the joining parts. Due do the extreme plastic deformation during the process, considerable changes in the microstructure in and around the weld seam take place. Normally this results in a very fine grained material, but in certain aluminium alloys like e.g. Al2195 subsequent heat treatments, sometimes only in combination with a precedent low temperature deformation can cause extreme anomalous grain growth. In this presentation results from metallographic analysis of samples showing such anomalous grain growth are shown. The onset can be controlled by the degree of precedent deformation, but also by welding parameters and by addition of further elements into the weld seam.

MM 7.3 Mon 12:15 H 0106

Influence of the heat treatment on the precipitation behavior on age-hardenable commercial Al-based alloys AA2195. — •Muna Khushaim[1], Judith Seibert[2], Ferdinand Haider[2], and Talaat Al-Kassab[3] — [1]Physical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia. — [2]University Augsburg, Inst. f. Physics, D - 86159 Augsburg, Germany. — [3]D-37077, Göttingen, Germany.

Many aluminum age-hardenable alloys have a good combination of strength and formability and exhibit an attractive enhanced strength/weight ratio. The enhancement of the mechanical properties has largely been attributed to the formation of different precipitates such as: T_1 (Al_2CuLi), $\theta^{'}$ (Al_2Cu), $\delta^{'}$ (Al_3Li) and $\beta^{'}$ (Al_3Zr).The object of this work is to investigate the dependency of the precipitation kinetics on the performed heat treatment conditions. Aluminum-Lithium - copper alloy AA2195 was selected as a model system in the present study. Common industrial heat treatments such as: T8 temper, T4 temper and T6 temper have been examined. Results are obtained by utilizing transmission electron microscopy (TEM), micro-hardness Vickers measurement, differential scanning calorimetry (DSC) and atom probe tomography (APT). In this contribution a detailed analysis of the correlation between the microstructure developments owing to the respective treatment condition and the hardening process will be presented.

MM 7.4 Mon 12:30 H 0106

Coherency and coarsening behavior of Al3(Sc,Zr) precipitation in aluminum alloys subjected to severe plastic deformation — •Vladislav Kulitckii[1], Sergey Malopheyev[1], Rustam Kaibyshev[1], Sergiy Divinski[2], and Gerhard Wilde[2] — [1]Laboratory of Mechanical Properties of Nanoscale Materials and Superalloys, Belgorod State University, Pobeda 85, Belgorod 308015, Russia — [2]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10 Münster, Germany

The coarsening behavior of the Al3(Sc,Zr) particles in Al-5.4Mg-0.4Mn-0.2Sc-0.09Zr (alloy 1) and Al-4.6Mg-0.35Mn-0.2Sc-0.09Zr (alloy 2) alloys was investigated using transmission electron microscopy (TEM). The alloys were subjected to equal channel angular pressing (ECAP) in the temperature range of 300-450°C and up a to total strain of ϵ~12. In the initial state, homogeneously distributed round nanoscale Al3(Sc,Zr) precipitates with average size ~9 nm were observed. Some of these particles featured a characteristic coffee-bean contrast, reflecting their coherence with the matrix. The severe plastic deformation of alloy 1 does not lead to significant coarsening of the Al3(Sc,Zr) particles, their average size was ~11 nm after ECAP at 300, 350, 400 and 450°C. Moreover, the coffee-bean TEM contrast was retained indicating the coherence between particles and matrix. In alloy 2, the Al3(Sc,Zr) precipitates demonstrated a different behavior. After deformation at 300-450°C, no significant change of the size of these precipitates was observed; however, some fraction of the particles lost their coffee-bean contrast and appeared as black circles.

MM 7.5 Mon 12:45 H 0106

Cluster model for precipitation in Al-alloys — •Tobias Stegmüller and Ferdinand Haider — Universität Augsburg, Inst. f. Physik, 86135 Augsburg

Precipitation processes in modern aluminum alloys are due to their signifance for mechanical properties of great technical interest. Proper choice of alloying elements in precipitation hardened alloys as well as an appropriate heat treatment allows to reach middle to high strength and to control corrosion resistance.

Despite the fact, that most of these processes are well understood both qualitatively and quantitatively, there is still a lack in a precise correlation between process parameters the resulting material properties. A key role for such a correlation can be formed by a precise model allowing to simulate the kinetics of a precipitation reaction.

One approach to model unmixing in binary alloys is the so-called dynamic cluster model. The basic idea is to describe the temporal evolution of the precipitate size distribution, starting from a supersaturated homogeneous solid solution. Mathematically, this means to solve an initial value problem: taking n as number of solute atoms in one particular cluster, c_n the concentration of clusters of size n, the temporal evolution is given by a master equation in terms of the respective probabilities for cluster growth and shrinkage of clusters containing n atoms.

In this work we present first results for an extended model for alloys with more than two components and with more complicated sequences of precipitate phases, as they occur in e.g. Al-Zn-Mg or Al-Cu alloys.

MM 8: Liquid and Amorphous Metals II: Structure Formation in Metallic Glasses

Time: Monday 11:45–13:00 Location: H 0107

MM 8.1 Mon 11:45 H 0107

On the path from disorder to long-range order in condensed matter — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

We well know how molecules form, but we are still lacking a deep understanding how long-range structural order is arising. Liquid and amorphous systems are predetermined to solve this situation. Both are following the completely disordered state and are precursors of the crystals. They should still show individual features of the elements involved, but should also show features of ordering. The emergence of medium-range order, as well as the correlated emergence and evolution of physical properties are in the focus of our research.

After the preparation of very different amorphous thin films we studied their structure and electronic transport properties over a large range of temperature and composition. In this contribution we will report on several involved scenarios, as well as new techniques to analyze the data, in particular the structural ones. We will report on pure elements, binary as well as ternary inorganic alloys, irrespective whether they are insulating or stay metallic. Our description will be the most simple to imagine, will deal with a few global species only, which themselves consist of collectively acting subspecies. Along this line we are able to reduce the tremendous number of parameters to describe e.g. 10^{23} individual atoms/ions to a few parameters only. Accordingly, we are able to understand the major structure-forming effects.

MM 8.2 Mon 12:00 H 0107

Non-isothermal crystallization kinetics of metallic glass by differential fast scanning calorimetry — •Bin Yang[1], Yulai Gao[2], and Christoph Schick[1] — [1]AG Polymer Physics, Institute of Physics, University of Rostock, Germany — [2]School of Materials Science and Engineering, Shanghai University, Shanghai, P.R. China

The thermal stability and the kinetic fragility of Al86Ni6Y4.5Co2La1.5 (%wt.) metallic glass were investigated by ultra-fast non-isothermal thermal analysis. The differential fast scanning calorimeter (DFSC) traces revealed that the material undergoes a three-stage crystallization for heating rates ranged from 5 to 40,000 K/s. Combining DSC and DFSC, the kinetics of the glass transition and crystallization of Al86Ni6Y4.5Co2La1.5 metallic glass was investigated. The kissinger plot can express the temperature dependence of growth rate of this metallic glass. Furthermore, the kinetic fragility for Al86Ni6Y4.5Co2La1.5 metallic glasses is evaluated. Depending on the fragility index, this metallic glass is a liquid of very high fragility, similar to several organics.

MM 8.3 Mon 12:15 H 0107

Effect of minor additions on the structure and dynamics of binary Zr-Cu melts — •Zach Evenson, Fan Yang, Dirk Holland-Moritz, and Andreas Meyer — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51147 Köln

The formation of bulk metallic glasses can be greatly enhanced through the minor addition of another element, although the underlying physical mechanisms remain largely unknown and often speculative. It has been suggested that minor additions can lead to a more sluggish melt kinetics as well as thermodynamically suppress competing crystal phases. However, very few studies are actually carried out in the melt to directly test these assumptions. We report on the effect of minor additions of Al and Ti on the structure, dynamics and glass-forming ability of binary Zr-Cu liquids. In order to accurately investigate the

physical properties of chemically reactive metallic melts and gain access to the metastable undercooled liquid, we employed electrostatic levitation (ESL) as a versatile containerless processing technique. Investigations of a $Zr_{50}Cu_{50}$ liquid with minor additions of only 4 at.% Al or Ti reveal a complex interplay between structure and dynamics as a result of chemical short-range order, extending beyond simple considerations based on free volume or atomic packing. The impact of minor additions on the glass-forming ability of this system is discussed in terms of non-ideal interactions between the melt constituents.

MM 8.4 Mon 12:30 H 0107

Effects of hydrogen-microalloying on the properties of bulk metallic glasses — •Davide Granata, Erwin Fischer, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland.

Microalloying, i.e. the addition of small amounts of alloying elements, has been found to be a viable tool to significantly improve the glass-forming ability (GFA) of metallic systems. In this work we identified hydrogen to be an ideal microalloying element to simultaneously improve the GFA and mechanical properties of bulk metallic glasses (BMGs). We processed various BMGs under a hydrogen-containing atmosphere and thus directly introduced hydrogen as an alloying partner to the resulting glass structure. Using this hydrogen-microalloying approach we found a simultaneous enhancement of the attainable critical casting thickness and malleability. The effectiveness of this processing route depends on how strongly hydrogen is incorporated into the microstructure and thus how strongly hydrogen (out-)diffusion can be suppressed. Based on these results, we will also discuss implications for future BMG design.

MM 8.5 Mon 12:45 H 0107

Influence of micro alloying on the bulk metallic glass former PdNiP — •Niklas Nollmann, Isabelle Binkowski, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität, Münster

When describing the deformation of bulk metallic glasses (BMGs), two different modes have to be distinguished. For high temperatures and low stresses homogeneous flow occurs, whereas for low temperatures and high stresses the flow becomes inhomogeneous. During inhomogeneous deformation of metallic glasses (e.g. in compression or bending) the strain is localized in thin regions, the so-called shear bands. In general, bulk metallic glasses show almost no ductility during plastic deformation. For instance, in compression tests BMGs fail catastrophically mostly at the location of one shear band that is typically inclined at about 45 degrees with respect to the load axis. The investigated PdNiP glass features a high ductility in bending compared to different metallic glasses. By the use of micro alloying, the mechanical properties of metallic glasses can be influenced. In our investigation, we demonstrate that the ductility in bending and compression of the PdNiP bulk metallic glass can be altered by adding small amounts of a differing element. Whereas cobalt additions improve the ability of plastic deformation, an iron addition leads to an almost complete loss of ductility. The results are discussed concerning the possible interrelation between minor alloying and plasticity enhancement.

MM 9: Hydrogen in metals II: Multiscale simulations

Time: Monday 11:45–13:15 Location: TC 006

Topical Talk MM 9.1 Mon 11:45 TC 006

Multiscale modeling of hydrogen-dislocation interaction — •Gerard Paul Leyson, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Straße 1, 40237 Düsseldorf, Germany

It has been well documented that hydrogen promotes embrittlement in a wide variety of materials. Despite the fact that the phenomenon is known for over a hundred years, the atomistic origin of hydrogen embrittlement is not well understood. One of the most promising models to explain hydrogen embrittlement is the Hydrogen Enhanced Local Plasticity (HELP) mechanism, which is based on the interaction between dislocations and hydrogen solutes. This mechanism has been well studied, but a quantitative connection between the hydrogen localization around dislocations and macroscopic embrittlement has yet to be achieved. To make this connection, we have developed a multi-scale model that can take into account the different length- and time-scale associated with the phenomenon, as well as takes into account the chemical interaction between hydrogen atoms. The hydrogen concentration profile generated by the model are in excellent agreement with direct atomistic simulations and predicts the correct relaxed dislocation core structure due to the formation of the nano-hydride, while being four orders of magnitudes faster. Direct connection with experiments was made by predicting the decrease in pop-in stress observed in hydrogen-charged nano-indentation experiments as a function of hydrogen chemical potential and temperature.

MM 9.2 Mon 12:15 TC 006

H-H interaction and critical temperature of hydride formation in palladium hydrogen thin films: Experiment and model — •Stefan Wagner and Astrid Pundt — University of Göttingen, Institute of Materials Physics

Palladium hydrogen (PdH) thin films are used as a model system to investigate the impact of elastic and microstructural constraints on structural phase transitions. Hydrogen-induced mechanical stress arises both from palladium film clamping on an elastically hard substrate and at coherent interfaces in the two-phase-coexistence region. It strongly changes the chemical potential of hydrogen, modifying the stability of the hydride phase. Mechanical stress is superimposed by microstructural constraints, channeling stress relaxation processes such as the formation of misfit dislocations in the films. In this paper we investigate hydrogen absorption and hydride formation in PdH thin films with different microstructure and clamping conditions [1]. The attractive H-H interaction energy and the critical temperature of hydride formation are determined quantitatively from the analysis of the chemical potential in combination with in situ stress measurement [2]. They differ for films with coherent interfaces and films where stress relaxation is possible. [1] S. Wagner, A. Pundt, Acta Mat. 59 (2011) 1862. [2] S. Wagner, M. Moser, A. Pundt et al., Int. J. Hydr. Energy 38 (2013) 13822.

MM 9.3 Mon 12:30 TC 006

Scale bridging modelling of hydride formation — •Robert Spatschek, Georgia Gobbi, Claas Hüter, Aurab Chakrabarty, Ugur Aydin, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Düsseldorf

We investigate phase separation in the bulk and at surfaces and find a reduction of the solubility limit near free surfaces due to elastic coherency effects. This mechanism favours nucleation from free surfaces even in the absence of external stresses. We apply the theory to hydride formation in nickel, iron and niobium and obtain a reduction of the solubility limit by up to two orders of magnitude at room temperature at free surfaces. This leads to a blurring of the distinction between hydride-forming and non-hydride-forming metals. Near stiff substrates, in contrast, the solubility limit is increased, in agreement with experimental observations. These effects are concisely expressed through a solubility modification factor, which transparently expresses the long-ranged elastic effects in a terminology accessible e.g. to ab initio calculations and experiments. The predictions are confirmed by Cahn-Hilliard simulations on the continuum level.

MM 9.4 Mon 12:45 TC 006

The Role of Temperature on the Free Energy of Hydrogen in Iron. — •Robert Horton and Michael Finnis — Royal School of Mines, Imperial College, London

A key advance in the development of hydrogen resistant steels is the inclusion of defects (such as vacancies and carbides) within the steel matrix to act as traps for the hydrogen. The development of predictive mesoscopic models to aid in the design of these steels requires knowledge of the chemical potentials of hydrogen both in the bulk and within the traps as a function of temperature.The high concentrations and high mobility of hydrogen in these systems brings the validity of traditional atomistic approaches to the calculation of the free energy into question.

In recent years a number of Monte Carlo techniques have been developed [1,2] that allow the calculation of the full partition function and thus the free energy of the system. These techniques provide

a promising route to calculating the free energy of systems containing high concentrations of defects [3].Through the application of these techniques to a system containing hydrogen in iron we show that they indeed allow one to calculate the free energy of such systems. Free energies calculated in this manner can then be included in mesoscale simulations.

[1]Wang, Fugao and Landau, D. P. (Mar 2001). Phys. Rev. Lett. (American Physical Society) 86 (10): 2050*2053. [2]Skilling, J.Bayesian Analysis 1, 833*860 (2006). [3]Horton, R. M. et al. Journal of Physics. Condensed matter 25, 395001 (2013).

MM 9.5 Mon 13:00 TC 006

Multiscale modelling of hydrogen embrittlement in metals — •Pratheek Shanthraj, Haiming Zhang, Gerard Leyson, Franz Roters, Tilmann Hickel, Dierk Raabe, and Jörg Neugebauer — Max Planck Institut für Eisenforschung, Düsseldorf, Germany

A multiscale phase field damage model is developed and coupled to a finite-strain thermo-mechanical framework to investigate the evolution of damage in metals under hydrogen-loaded conditions. The evolution of damage is based on the nucleation and growth of voids driven by the conservative transport and coagulation of hydrogen-stabilized superabundant vacancies, as well as the propagation of cracks driven by the competition between stored elastic energy at the crack tip and the hydrogen-dependent material decohesion energy. The dynamics of the hydrogen-decorated-vacancy concentration field and the damage microstructure is expressed in the form of a coupled Cahn-Hilliard and Allen-Cahn system of equations, respectively, and the physically based model parameters, such as decohesion and vacancy formation energies under hydrogen-loaded conditions, are obtained from ab-initio calculations, thus rendering the approach a multiscale modeling framework. As a case study, a polycrystalline aggregate, whose elasto-plastic mechanical response is governed by a local crystal plasticity model, is deformed under a range of hydrogen-loaded conditions to investigate the role of grain boundaries in the damage evolution process as a potential source and sink for vacancies as well as a site for interface decohesion.

MM 10: Functional materials II: Battery Materials

Time: Monday 11:45–13:00 Location: TC 010

MM 10.1 Mon 11:45 TC 010

Towards an All-Solid-State Thin-Film Li-Ion Battery by Novel CO2-Laser Assisted Chemical Vapor Deposition — •Christoph Loho[1], Azad Darbandi[1,2], Ruzica Djenadic[1,3], Oliver Clemens[1,2], and Horst Hahn[1,2,3] — [1]Joint Research Laboratory Nanomaterials, Technical University of Darmstadt and Karlsruhe Institute of Technology, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]Helmholtz Institute 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, which drives the current research on thin-film batteries. Among the applications are RFID tags, pacemakers, energy harvesting and lab-on-a-chip devices. 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. Regarding fabrication, chemical vapor deposition (CVD) is a suitable method to grow functional thin-films for Li-ion batteries, since it allows for a homogeneous growth over large areas with high deposition rates and a very high purity. Unique is also the capability of conformal, directional deposition in order to realize three-dimensional architectures. In this contribution we report on our latest progress towards an all-solid-state thin-film Li-ion battery deposited by novel CO2-laser assisted chemical vapor deposition (LA-CVD). The detailed characterization of (i) LiCoO2 and (ii) Li7La3Zr2O12 thin-films includes results on microstructure, phase composition and electrochemical performance.

MM 10.2 Mon 12:00 TC 010

Modeling the structural stability during delithiation in Li-Mn-Ni oxides from first-principles — •Jan-Michael Albina, Anika Marusczyk, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The gradual reduction in both the charge and discharge voltage upon cycling in lithium batteries (aka voltage fade) is related to phase transformations in the cathode material. Therefore a better understanding of the phase transformation sequences occurring during cycling is important for improved performance of cathode materials. In this work we present a first-principles approach for modeling and analyzing phase relationships in multi-component systems. In particular, we will study the effect of delithiation on the phase evolution, phase stability, and variation of the chemical potentials for a selection of cathode materials based on Li-Mn-Ni oxides. The open circuit voltage will be estimated and discussed.

MM 10.3 Mon 12:15 TC 010

Single crystal growth, magnetism and ionic conductivity of $LiMn_{1-x}Fe_xPO_4$ — •Christoph Neef[1], Hubert Wadepohl[2], Hans-Peter Meyer[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg — [2]Anorganisch-Chemisches Institut, Universität Heidelberg, D-69120 Heidelberg — [3]Institut für Geowissenschaften, Universität Heidelberg, D-69120 Heidelberg

Single crystals $LiMn_{1-x}Fe_xPO_4$ were grown using the optical floating zone technique at elevated argon pressure up to 30 bar. The resulting mm-sized single crystals were used to study the influence of Fe doping on the structural, magnetic and transport properties by means of single crystal XRD, thermal expansion, magnetometry, and impedance spectroscopy. The resulting phase diagram illustrates the evolution of the long range antiferromagnetically ordered ground state for different doping levels. The ionic conductivity which is of particular interest for application of the material in Li-ion batteries is very low in the end member $LiMnPO_4$ but clearly increases upon Fe doping.

MM 10.4 Mon 12:30 TC 010

A Mn3O4@MWCNT composite as anode material for Li-ion batteries — •Alexander Ottmann[1], Philip Schneider[1], Elisa Thauer[1], Maik Scholz[2], Marcel Haft[2], Markus Gellesch[2], Franziska Hammerath[2], Bernd Büchner[2], Silke Hampel[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany

Mn_3O_4 nano-sized particles have been incorporated into the inner hollow cavities of multi-walled carbon nanotubes (MWCNT) via a solution-based approach. The resulting composite material with about 40 $wt\%$ of incorporated Mn_3O_4 has been used for electrochemical half-cell studies against Li^0/Li^+ by means of cyclic voltammetry and galvanostatic cycling with potential limitation (GCPL). For electrode preparation, no additional carbon black has been used. Cyclic voltammetry shows well-performing working electrodes. The redox peaks during the first half-cycle indicate formation of MnO and subsequently its reversible conversion reaction to metallic Mn. This is confirmed, e.g., by our magnetic studies. In addition, the electrochemical data reveal the formation of a solid electrolyte interface (SEI) and reversible lithium de/-intercalation into the MWCNT. The GCPL data confirm complete conversion of Mn_3O_4 to MnO during the first half-cycle and full accessibility of the theoretical capacity of the $MnO + 2Li^+ + 2e^- <=> Li_2O + Mn$ conversion reaction (703 $mAhg^{-1}$). The composite material reaches a maximum discharge capacity of 461 $mAhg^{-1}$ at a current of 100 mAg^{-1} and maintains 97% of it in the 30^{th} cycle.

MM 10.5 Mon 12:45 TC 010

Separation of surface and bulk stress in a model lithium alloy electrode reveals grain boundary alloying at high electric potentials vs. Li/Li+. — •Tobias Kitzler[1], Jürgen Markmann[1,2], Emad Maawad[3], Daniel Többens[4], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Department of Materials Reserch, Materials Mechanics — [2]Hamburg University of Technilogy, Department of Materials Physics and Materials Technology — [3]Helmholtz-Zentrum Geesthacht, Department of Materials Reserch, Materials Physics — [4]Helmholtz-Zentrum Berlin, Department of crystallography

We present the results of a combined study using the potential strain coupling parameter and microstructural characterisation to separate surface and bulk contributions to the stress in gold thin film electrodes

during electrochemical cycling in an organic lithium electrolyte.

The results were used to show, that grain boundary alloying is an important mechanism which appears long before intermetallic alloys appear, and that it induces a stress on a film electrode which can easily be mistaken as a surface stress. This is especially important, since the effect is in the same order of magnitude (apparent surface stress: -2.9 N/m) as the actual surface stress. Furthermore the separation allowed estimating the surface stress resulting from underpotential deposition of lithium on the gold surface of roughly -2.6 N/m, which is good agreement with DFT results of -2.8 N/m calculated by Tavessol et. al.

MM 11: Biomaterials and Biopolymers I (joint BP/CPP)

Time: Monday 14:30–17:15 Location: EB 202

MM 11.1 Mon 14:30 EB 202

Determination of Conformational Entropy of Fully and Partially Folded Conformations of Holo- and Apomyoglobin — •Andreas Stadler[1], Marek Koza[2], and Jörg Fitter[3,4] — [1]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Institut Laue-Langevin, CS 20156, 38042 Grenoble, France — [3]Institute of Complex Systems (ICS-5): Molecular Biophysics, Forschungszentrum Jülich GmbH, 52425 Jülich — [4]I. Physikalisches Institut (IA), AG Biophysik, RWTH Aachen, Sommerfeldstrasse 14, 52074 Aachen

Holo- and apomyoglobin can be stabilized in native folded, partially folded molten globules (MGs) and denatured states depending on the solvent composition. In a comparative experimental study we investigated the correlation between protein folding and dynamics on the picosecond time scale using incoherent quasielastic neutron scattering (QENS). The conformational entropy difference ΔSconf between the folded conformations and the acid denatured state could be determined from the measured mean square displacements and was compared to the entropy difference ΔS obtained from thermodynamic parameters. The observed difference between ΔS and ΔSconf was attributed to the entropy difference ΔShydr of dynamically disordered water molecules of the hydration shell. The entropy content of the hydration water is significantly larger in the native folded proteins than in the partially folded MGs. We demonstrate the potential of incoherent neutron scattering for the investigation of the role of conformational dynamics in protein folding.

MM 11.2 Mon 14:45 EB 202

Mechanical rupture of mono- and bivalent coordination compounds — •Manuel Gensler[1], Christian Eidamshaus[2], Arthur Galstyan[2], Ernst-Walter Knapp[2], Hans-Ulrich Reissig[2], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]Institute of Chemistry and Biochemistry, Freie Universität Berlin

Biomolecular systems are commonly exposed to a manifold of forces, often acting between multivalent ligands. To understand these forces we studied a monovalent and three bivalent pyridine Cu(II) coordination complexes with varying backbone structures. We performed SFM based single-molecule force spectroscopy in aqueous environment and compared results with ab-initio DFT calculations. According to the Kramers-Bell-Evans theory, all interactions show remarkably long rupture lengths of more than 3 Å. We explain this observation by dissociation mechanisms involving hydrogen-bound intermediate states. Additionally we show that most probable rupture forces of the bivalent systems can be larger, but also smaller than those of the monovalent counterpart. In contrast, when our results are extrapolated to forceless conditions, all bivalent systems show lower thermal off-rates. The mechanical stability is not solely determined by binding energy, but also by rupture lengths. Thus both parameters should be considered in the rational design of biomolecular ligands.

MM 11.3 Mon 15:00 EB 202

Opposite translocation of long and short oligomers through a nanopore — •Thomas Töws, Sebastian Getfert, and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We consider elongated cylindrical particles, modeling e.g. DNA fragments or nano-rods, while translocating under the action of an externally applied voltage through a solid-state nanopore. Particular emphasis is put on the concomitant potential energy landscape due to the complex interplay of various electrohydrodynamic effects beyond the realm of small Debye lengths. We find that the net potential energy difference across the membrane may be of opposite sign for short and long particles of equal diameters and charge densities (e.g. oligomers). Thermal noise thus leads to biased diffusion through the pore into opposite directions. The specific particle length at which this transport inversion occurs can be controlled by means of a membrane gate electrode.

MM 11.4 Mon 15:15 EB 202

Hydrodynamic Slip on DNA in Nanopore Translocation Experiments — Lukas Galla[1], •Andreas J. Meyer[1], Andre Spiering[1], Andy Sischka[1], Michael Mayer[2], Adam R. Hall[3], Peter Reimann[1], and Dario Anselmetti[1] — [1]University of Bielefeld, Germany — [2]University of Michigan, USA — [3]Wake Forest University School of Medicine, USA

In a recent paper, we reported on the observation of hydrodynamic slip on DNA by optical tweezers-controlled translocation experiments in solid-state and lipid-coated nanopores [1]. After a short introduction to the performed experiments, I will present our theoretical model describing the dominating electrohydrodynamic effects, with particular emphasis on the hydrodynamic slip boundary condition.

By solving the Poisson-Nernst-Planck and Stokes equations using finite element methods it is possible to gain insight into the influence of nanopore geometry and composition on translocation experiments. Furthermore, these continuous models of electrohydrodynamics can serve as an appropriate basis for dynamic DNA simulations.

[1] L. Galla, A. J. Meyer, A. Spiering, A. Sischka, M. Mayer, A. R. Hall, P. Reimann, and D. Anselmetti (2014). Hydrodynamic slip on DNA observed by optical tweezers-controlled translocation experiments with solid-state and lipid-coated nanopores. Nano Letters, 14(7), 4176-4182.

MM 11.5 Mon 15:30 EB 202

How to escape the maze — •Teresa Behl[1], Felix Höfling[2], and Thomas Franosch[3] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität, München — [2]Max Planck Institute for Intelligent Systems, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [3]Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Austria

Recently, novel materials such as carbon nanotubes extended the interest in the diffusion dynamics of semiflexible polymers far beyond classical biophysics. Semiflexible polymers form entangled networks when dispersed in solution by virtue of their lengthy nature. Due to their relative stiffness they exhibit a reptation movement to escape their local surrounding maze of crossing polymers, usually modelled as a tube constraining the polymer sterically.

We have investigated the dynamics of a semiflexible polymer via computer simulations of a 2D bead-rod-algorithm. Point obstacles mimic the cross sections of the surrounding polymers with the plane in which the polymer diffuses. Extensive computer simulations are performed to resolve the slow disentanglement processes. In particular we measure the translational and rotational diffusion for a broad density range. Furthermore, we discuss the intermediate scattering function and the chances and limitations of the performed simulations.

15 min break

MM 11.6 Mon 16:00 EB 202

Theory on linear viscoelasticity of a cytoskeletal network — •Tetsuya Hiraiwa and Roland Netz — Freie Universität Berlin, Germany

Mechanical properties of a cortical cytoskeleton, which is a network consisting of actin filaments and crosslinker proteins located underneath the cell membrane, govern the elastic and viscous resistances of

living cells to deformation and are crucial for wide variety of cellular functions. I would like to present a theoretical method to evaluate linear viscoelasticity of a filamentous network like a cortical cytoskeleton based on properties of single segments. Using the method, we can explain a universal power-law in complex moduli, which is also found in several experiments and our numerical simulation.

MM 11.7 Mon 16:15 EB 202

Scaling with persistence length: Expanding the accessible phase space of semi-flexible polymer networks via DNA tubes — •Carsten Schuldt[1,2], Jessica Lorenz[2], Jörg Schnauss[1], Tina Händler[1], Martin Glaser[1], Josef A. Käs[1], and David M. Smith[2] — [1]University of Leipzig, Soft Matter Physics Division, Leipzig, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany

Biologically evolved materials are often used as inspiration in both the development of new materials as well as examinations of underlying physical principles governing their general behavior. One prominent example is actin and its set of accessory proteins. However, a major limitation lies in the molecular toolbox provided by naturally occurring biological systems. The inability to deterministically modulate or "program" basic properties such as stiffness or interaction strengths hinders a meticulous examination of the parameter space, and the subsequent potential for developing new classes of materials.

We overcome these limitations emplyoing model systems assembled from programmable nanomaterials such as DNA. Nanotubes with similar dimensions and mechanical properties as actin filaments can be constructed from small sets of specially designed DNA strands. Properties such as stiffness and inter-filament attraction (i.e. crosslinking) can be controlled through the design of a particular set of DNA strands. Forming networks from these semi-flexible polymers, we test established theories with respect to these parameters for the first time.

MM 11.8 Mon 16:30 EB 202

pH-dependent Ordered Fibrinogen Adsorption on Polyethylene Single Crystals — •Christian Helbing[1], Robert Schulze[1], Dominik Hering[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto-Schott-Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Jena, Germany — [2]Clemenshospital Münster, Münster, Germany

The biological performance of materials is mostly determined by protein adsorption at the biomaterials surface. Nanostructured surfaces can influence the assembly and orientation of adsorbed proteins. The aim of the current study was to control the protein adsorption by nanostructured surfaces. For this, we tested the hypothesis that human plasma fibrinogen (HPF) assemblies can be oriented on the (001) surface nanostructures of Polyethylene Single Crystals (PE-SC).

At a physiological pH of 7.4, HPF assemblies consisted of crosslinked HPF molecules, e.g., protofibrils, networks or sponge-like structures in dependence of the protein concentration. However, at an increased pH of 9.2 spherical-shaped and trinodal-shaped single HPF assemblies were observed. The observation of these multi protein assemblies (pH 7.4) and the single HPF assemblies (pH 9.2) can be explained by activated (pH 7,4) and deactivated (pH 9.2) HPFs αC-domains. While the single trinodal-shaped HPF molecules preferred an orientation along crystallographic [100] and [010] directions on the nanostructured PE-SC surface the HPF protofibrils showed no preferential orientation. The current study deepens the understanding of controlled protein assembly and orientation on nanostructured surfaces.

MM 11.9 Mon 16:45 EB 202

Insights into diatom biomineralization with nanoscale silica-peptide hybrid films — •Helmut Lutz[1], Vance Jaeger[2], Jim Pfaendtner[2], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max-Planck-Institute for Polymer Science, Mainz — [2]University of Washington, Chemical Engineering, Seattle

Taking clues from diatom silification we have recently shown that amphiphilic peptides consisting of lysine and leucine (LK peptides) are capable of producing silica wires, spheres and tubes, depending on their secondary structure. Precipitating particles, i.e. mineralization in three dimensions is very different from the two dimensional silification required for the cell walls of diatoms. Hence, we studied mineralization in 2D at the air-water interface. At the interface, slightly different peptides can adopt alpha helical or beta sheet structures depending on the hydrophobic periodicity of amino acids. Upon addition of a silica precursor we were able to obtain peptide-silica hybrid films with a thickness of ~4 nm. By means of surface sensitive techniques, such as sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS) we were able to probe the film composition and interactions between peptides and silica at the early stages of biomineralization. Electron and atomic force microscopy show that the fine structure of the film resembles the in-solution silica precipitates of each peptide. We employed molecular dynamics simulation techniques to complement the experimental insights with a computational model. Our results provide insights into the biomineralization of structured films, which might prove useful in materials design and surface engineering.

MM 11.10 Mon 17:00 EB 202

Mapping internal mineral strains in human dentine under tension: X-ray diffraction insights into the contribution of the mineral nano-particles to the load-bearing capacity of tooth tissue. — Jean-Baptiste Forien[1], •Claudia Fleck[2], Peter Fratzl[3], and Paul Zaslansky[1] — [1]Julius Wolff Institut, Berlin, Germany — [2]Technical University, Berlin, Germany — [3]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Teeth are hierarchical strong and stiff structures, consisting of a mineralized protein-based composite (dentine). They function under mechanical load, and the nanometer-sized hydroxyapatite mineral particles in the collagen fiber matrix deform as a response to applied external stress (Deymier-Black,2012). In this study, we report on the mineral response in human dentine to mechanical tensile testing. We track mineral particles following changes in the mineral dimension using X-ray diffraction. It is thus possible to compare the stresses experienced by the mineral particles with the stress applied by the external load. We find that the tissue to mineral strain ratios observed increase until they reach a value of 2, which is three times lower than for bone (Gupta,2006), and suggests that a different load-partitioning mechanism exists in teeth. We also find that the Poisson's ratio decreases with increasing load, suggesting that as load increases, there is some dynamic change in the loads transferred to the crystals, similar to what was found for bovine dentine loaded in compression. With increasing load, more strain-energy is orientated along the tensile axis and less is distributed into particles oriented along other orientations.

MM 12: Invited talk Pyczak

Time: Monday 15:00–15:30 Location: TC 006

Invited Talk MM 12.1 Mon 15:00 TC 006

Insights into phase transformations and microstructure development of TiAl alloys by use of advanced characterisation techniques — •Florian Pyczak — Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

γ-TiAl alloys, which started out as two phase materials based on the binary Ti-Al phase diagram. Due to the addition of increasing amounts of alloying elements for property optimisation the materials became more and more complex. Frequently not only properties but also the phase constitution is altered. The characterisation of these additional phase constituents with respect to their structure, formation paths, morphology development and integration in the microstructure is an attractive application field for advanced characterisation methods. High energy X-ray diffraction (HEXRD) at synchrotron sources allows the direct observation of phase transformations at temperature by the use of in-situ specimen environments. This is favourable as the high temperature phase constitution is often masked by subsequent lower temperature phase transformations. Also the transformation of one phase into another can be monitored on a grain by grain basis by these methods. The morphology development of precipitates, even if their size is just some nanometers, can be observed by high resolution electron microscopy picturing the interfaces between these precipitates and the TiAl matrix directly at the atomic scale. Thus, measurements at temperature, with high lateral resolution or by combination of different methods can provide a more complete picture of microstructure changes in the complex microstructures of these TiAl alloys.

MM 13: Microstructure and Phase Transformations III

Time: Monday 15:45–16:45 Location: H 0106

MM 13.1 Mon 15:45 H 0106

X-ray nanodiffraction with in situ load and pressure — •Christina Krywka[1], Angelika Zeilinger[2], Jozef Keckes[2], and Martin Müller[1] — [1]Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, Geesthacht D-21502 — [2]Montan-Universität Leoben, Dep. Materialphysik, Jahnstraße 12/I, A-8700 Leoben

Scanning X-ray nanodiffraction (SXND) is an excellent tool for materials science. It readily serves structural information with submicrometer spatial resolution from crystalline and semi-crystalline materials, suitable to retrieve residual stress microprofiles or crystal structure. Provided a sufficiently high energy and long focal distance, SXND experiments can be performed on metallic samples and in extended sample environments, making SXND of course a highly desirable method for materials science.

SXND experiments were performed with a beam size of 350 nm * 250 nm with in situ high pressure application and with in situ nanoindentation, using homebuilt sample environments and the conditions at the Nanofocus Endstation of beamline P03 (PETRA III, Hamburg). A hydrostatic pressure cell was used in combination with a 19 keV nanobeam for the first time in order to record spatially resolved data from a fractured silver sample at (truly isotropic) hydrostatic conditions below 1 GPa. The nanoindentation setup on the other hand was used to apply directed strains of similar magnitude onto microstructured Ti-Al hard coatings at 15 keV in order to observe processes inducing fracture of the coating.

MM 13.2 Mon 16:00 H 0106

Illuminating Correlative Research using X-ray and Electron Microscopy — •Lars-Oliver Kautschor[1], Arno P. Merkle[2], Jeff Gelb[2], and Lorenz Lechner[2] — [1]Carl Zeiss Microscopy GmbH, Oberkochen, Germany — [2]Carl Zeiss X-ray Microscopy, Inc., Pleasanton, CA USA

X-ray tomography has emerged as a new powerful imaging technique that obtains 3D structural information from opaque samples under a variety of conditions and environments. It has rapidly become an accepted laboratory technique offering quantitative information in the materials sciences. We present ways in which non-destructive 3D volumetric information, obtained via laboratory nanoscale and sub-micron X-ray microscopy (XRM) are increasingly used to probe scientific questions as a complement to Electron- and Light-based microscopy methods. These correlative methods, relating to XRM, provide an opportunity to study materials evolution at multiple length scales in 3D and utilize this information to inform or guide postmortem analysis to be most efficient.

In materials research, the motivation to correlate XRM information with postmortem EM stems from different primary reasons. XRM is used as a 3D navigation system ("Google Earth" in 3D) for targeting and finding specific buried structures of interest for extraction or cross sectional imaging. We demonstrate several examples, including energy materials, automotive applications and metals, upon which the use of XRM and FIB/SEM information on the same specimen has contributed to a more complete understanding of a materials system.

MM 13.3 Mon 16:15 H 0106

In situ investigation of the microstructure in friction stir welded steels usind high-energy X-ray diffraction — •Malte Blankenburg, Peter Staron, Andreas Stark, Torben Fischer, Daniel Laipple, Norbert Schell, Jakob Hilgert, 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. With a fast area detector, time-resolved measurements with image rates up to 10 Hz were possible, delivering detailed insight to the time development of the ferrite and austenite content of small gauge volumes at different positions relative to the welding tool. Post-mortem EBSD analysis of weld profiles were performed to confirm the results of the *in situ* welding experiments. Additionally, the phase transformations in the steels used for friction stir welding were studied with a dilatometer (DIL805 A/D) in the synchrotron beam.

MM 13.4 Mon 16:30 H 0106

Thermodynamics of point defects and diffusion mechanisms in B2-ordered compounds — •Michael Leitner — Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

A scheme to classify the point defect thermodynamics in B2 compounds by way of two non-trivial energy parameters is presented, which is rigorously valid for small defect concentrations in both stoichiometry and off-stoichiometry. It is applied to published ab initio defect formation energies, and the variety of resulting phenomena is demonstrated. Further, by introducing model assumptions the consequences for the active diffusion mechanisms are deduced. It is shown that particularly for the case of off-stoichiometry, the assumed prevalence of either the six-jump cycle or the triple defect mechanism has to be reconsidered, as two qualitatively different mechanisms emerge as likely candidates for the dominant effect.

MM 14: Transport I: Diffusion

Time: Monday 15:45–17:45 Location: H 0107

MM 14.1 Mon 15:45 H 0107

Diffusion of solutes in Ni-based superalloys: role of vacancies and the treatment of the non-dilute limit — •Sergej Schuwalow, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

High-temperature properties of Ni-base superalloys are known to be highly dependent on the alloying additives, in particular on the presence of Re. Current knowledge of the mechanisms behind this effect is mostly phenomenological in nature and the details of solute diffusion, interaction with various defects (e.g. interfaces, vacancies, and dislocations) as well as the interplay between composition and microstructure are not well understood.

We have analyzed concentration/temperature-dependent diffusion behavior of selected alloying elements in the dilute limit using a combination of density-functional theory calculations and kinetic Monte Carlo simulations [1]. We found that the diffusion of vacancies, which was speculated to be at the core of the Re effect in literature, is only weakly influenced by the presence of the solute elements at concentrations below 3wt%.

At higher solute concentrations solute-solute interactions need to be taken into account. Here we present developments on a cluster expansion approach for non-dilute systems which allows an ab-initio treatment of diffusion in presence of configurational disorder. We further discuss avenues for the treatment of multicomponent systems.

[1] S. Schuwalow, J. Rogal, R. Drautz, J. Phys.: Condens. Matter 26 (2014) 485014.

MM 14.2 Mon 16:00 H 0107

Phase composition, microstructure and Ni tracer diffusion in FCC FeCrCoNi-based high entropy alloys — •Mayur Vaidya[1,2], Simon Trubel[2], Igor Golovin[3], Buduraju Srinivasa Murty[1], Sergiy Divinski[2,3], and Gerhard Wilde[2] — [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India — [2]Institute of Material Physics, University of Muenster, Muenster, Germany — [3]National University of Science and Technology MISiS, Moscow, Russia

High entropy alloys (HEAs) CoCrFeNi, CoCrFeMnNi and CoCrFeMnNiV were prepared by arc melting the constituent elements, followed by homogenization at 1200°C for 50 h. XRD results show that CoCrFeNi and CoCrFeMnNi represent single phase FCC phases, while CoCrFeMnNiV comprises of FCC and tetragonal phases. EBSD analysis confirms a single phase structure, uniform composition and a grain size in excess of 250μm in CoCrFeNi and CoCrFeMnNi alloys. Elemental X-ray maps of CoCrFeMnNiV substantiate its decomposition into a Ni- and Mn-rich phase (located predominantly at grain boundaries) and a V- and Cr-rich phase. Such FCC-HEAs have been explored for high temperature applications, for which creep behavior and in turn the diffusion kinetics of these alloys must be understood. We are studying Ni tracer diffusion in these HEAs using ^{63}Ni radioisotope. Ni diffusion kinetics, amplitude- and temperature dependent mechanical damping in HEAs are reported. Partial support by the Ministry of Education and Science of Russia in the framework of Increase Competitiveness Program of NUST MISiS(K3-2014-045) is acknowledged.

MM 14.3 Mon 16:15 H 0107

Investigating the effect of severe plastic deformation on nickel using radiotracer diffusion and microstructural analysis — •Simon Trubel[1], Sergiy Divinski[1], Martin Peterlechner[1], Gerrit Reglitz[1], Matthias Wegner[1], Christian Simon[1], Ehud Almog[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik der WWU, Münster, Deutschland — [2]Technion, Haifa, Israel

Ultrafine grained and nanocrystalline materials produced by methods of severe plastic deformation (SPD) have roused a growing interest in science and technology. Previous experiments on Nickel of 99.6% purity revealed ultra-fast diffusion rates in ultrafine grained material severely deformed via equal channel angular pressing (ECAP) [1] and high pressure torsion (HPT). This study reports the effect of pre-annealing of ECAP-processed Ni on the grain boundary characteristics and the thermal stability of microstructure. Grain boundary self-diffusion has been analysed using the 63Ni radioisotope in combination with high-precision parallel grinding. The results of the diffusion measurements and of measurements by electron backscattered diffraction (EBSD) and transmission electron microscopy (TEM) are discussed with respect to modifications of grain boundary structures under different routes of SPD processing. Additionally, cold rolled Nickel is investigated as another variant of severely deformed material that has been processed along a different deformation pathway in order to gain insight into the formation conditions of the grain boundaries that act as ultra-fast diffusion paths after SPD treatment. [1] S. V. Divinski, G. Reglitz, H. Rösner, Y. Estrin, G. Wilde. Acta Materialia, 59, 1974 (2011).

MM 14.4 Mon 16:30 H 0107

Kinetics and structural effects induced by liquid Ga penetration into ultra-fine grained Al — •Mehrnoosh Naderi, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

One of the spectacular examples of liquid metal embrittlement is the fast penetration of liquid gallium into aluminum and its alloys which occurs even at room temperature, i.e. below the melting point of Ga. Since severe plastic deformation is commonly used for grain refinement and produces a high density of grain boundaries of different types, in this study we focus on the penetration of Ga along grain boundaries of ultra-fine grained Al produced by high pressure torsion (HPT). The volumetric changes and the kinetics of liquid Ga penetration into the Al grain boundary network are investigated. A two-stage process of the excess volume evolution in HPT-processed Al is observed after Ga application. The structural effects are examined by transmission electron microscopy and texture measurements, too. The surface evolution is followed by atomic force microscopy. The results are discussed concerning the underlying mechanisms that control the Ga penetration.

15 min. break

MM 14.5 Mon 17:00 H 0107

Microstructure and Stress Relaxation in Thin Nano Crystalline Platinum Films — •Wolfgang Gruber[1], Florian Strauss[1], Lars Dörrer[1], Michael Horisberger[2], Thomas Geue[2], Jochen Stahn[2], Carsten Bähtz[3], and Harald Schmidt[1] — [1]TU Clausthal, Institut für Metallurgie — [2]Paul Scherrer Institut, Laboratory for Neutron Scattering — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung

Various techniques can be used to deposit thin metal films with a thickness in the nanometer range on a substrate. Independent of the method of production residual stress is present in the metal films after deposition. Based on the concept of dilatometry X-ray diffraction and X-ray reflectometry was used to investigate the correlation of strain relaxation and the change of point defect concentration in thin Pt films [1]. In the present work in-situ measurements using synchrotron radiation were performed in the temperature range between 100 °C and 300 °C to investigate strain relaxation in thin Pt films deposited on oxidised silicon substrates via magnetron sputtering and ion beam sputtering, respectively. Self-diffusion of Pt was investigated for samples produced by ion beam sputtering using secondary ion mass spectrometry and neutron reflectometry. The two systems are compared taking the microstructure as revealed by X-ray analysis into account.

W. Gruber, S. Chakravarty, C. Baehtz, W. Leitenberger, M. Bruns, A. Kobler, C. Kübel, H. Schmidt, Phys. Rev. Lett. 117 (2011) 265501.

MM 14.6 Mon 17:15 H 0107

Multiscale modeling approach to occupationally disordered materials: Ion diffusion in Lithium-Titanium-Oxide battery materials — •Hendrik H. Heenen, Saskia Stegmaier, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Lithium-titanium-oxide (LTO) materials have caught a lot of attention as an alternative anode material for lithium ion batteries as they offer high cycling stability, safe operation at high working potentials and a fast charge-discharge behavior. Aiming to link this macroscopic electrochemical performance to the underlying atomic-scale processes, first-principles studies generally offer a unique opportunity to understand the Li ion diffusion and material's structure. In particular for the spinel-type $Li_4Ti_5O_{12}$ LTO they are, however, challenged by the mixed occupancy of octahedral sites by Li and Ti ions [1]. This allows for a high degree of occupational disorder that can not be appropriately

sampled within supercell sizes accessible to present-day first-principles calculations. We address this challenge with a multiscale approach involving interatomic potentials that are parametrized and validated by density-functional theory. This allows to thoroughly sample the configuration space of $Li_4Ti_5O_{12}$ and perform an analysis of the variety of diffusion pathways. Particular focus is placed on the dependency of the average and local Li ion mobility on the thermodynamically accessible configuration space.

[1] B. Ziebarth *et al*, Phys. Rev. B **89**, 174301 (2014).

MM 14.7 Mon 17:30 H 0107

Self-Diffusion in Amorphous Silicon Investigated by Neutron Reflectometry — •Florian Strauss[1], Harald Schmidt[1], Jochen Stahn[2], and Thomas Geue[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Paul Scherrer Institut, Villigen, Schweiz

The characteristics of silicon self-diffusion in the amorphous state are still unknown, albeit the material is widely used in solar cells, flat screen displays and is looked at as a promising electrode material in Li-ion batteries. In this model system of a covalent amorphous semiconductor low diffusivities and intrinsic metastability necessitate the use of Neutron Reflectometry (NR) a method capable of determining diffusion lengths of 1 nm and below [1,2]. $^{29}Si/^{28}Si$ isotope multilayer structures are prepared by ion beam sputtering and thermally treated in an Ar atmosphere at temperatures up to 700 °C in order to induce isotope-interdiffusion. The chemical homogeneity and amorphous structure are confirmed by cross-sectional TEM measurements and XRD data. At temperatures between 350 and 500 °C a time dependent short range diffusion process on the length scale of 1 nm is observed and interpreted as a consequence of structural relaxation. At temperatures above 500 °C diffusion over a range of several nanometres is found. Additional measurements by Secondary Ion Mass Spectrometry confirm the data obtained by NR.

[1] H. Schmidt et al., Acta Mater. 56 (2008), 464
[2] E. Hüger et al., Appl. Phys. Lett. 93 (2008), 162104

MM 15: Hydrogen in metals III: Experiments

Time: Monday 15:45–18:00 Location: TC 006

Topical Talk MM 15.1 Mon 15:45 TC 006

On the combination of different experimental techniques to increase understanding on the hydrogen/material interaction in iron based alloys — Tom Depover, Elien Wallaert, Aurélie Laureys, Emilie Van den Eeckhout, and •Kim Verbeken — Ghent University, Department of Materials Science and Engineering, Technologiepark 903, B-9052 Ghent (Zwijnaarde)

Hydrogen induced cracking might arise when metals are in contact with an H-containing environment. Although known for a long time, the explanation of the responsible mechanism still remains under discussion. New, high strength metals appear more prone to H-related failure. The microstructure complexity of such metals even complicates the study of H induced phenomena. Moreover, H interacts in a very specific way with each microstructural feature. Furthermore, H-related research is a very challenging task due to the low H solubility, high H mobility and difficult H visualization.

H-material interactions can be studied via evaluating the effect of hydrogen on the mechanical properties, done by tensile tests after or during charging, characterizing H trapping via thermal desorption spectroscopy, studying H diffusion by electrochemical permeation and advanced characterization of H-induced cracks by electron backscatter diffraction. In this work, an overview is given on some recent results on the H-material interactions in iron-based alloys by combining these techniques. It will be demonstrated that the combination of these data is an asset contributing to the elucidation of the complicated H-material interactions.

MM 15.2 Mon 16:15 TC 006

Hydrogen diffusivity as a measure for relative dislocation densities in palladium — •Martin Deutges[1], Hans Peter Barth[2], Yuzeng Chen[3], Christine Borchers[1], and Reiner Kirchheim[1,4] — [1]Institut für Materialphysik, Georg-August Universität Göttingen — [2]Now at: DLR Göttingen — [3]State Key Lab of Solidification Processing, Northwestern Polytechnical University, Xi'an, P.R. China — [4]International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan

It is well known that hydrogen affects the defect formation energy [1] which is thermodynamically described by the defactant concept [2]. The palladium-hydrogen system was chosen to analyze the effect of hydrogen on the formation of dislocations [3,4]. For this purpose palladium was loaded with different amounts of hydrogen and subsequently cold rolled. The dislocation density was quantified by measuring hydrogen diffusivity, which depends on the amount of trap sites for hydrogen. The results were compared to conventional XRD-methods [4]. After cold rolling, residual hydrogen is removed. During reloading with hydrogen the diffusion through the material is measured. The change in diffusivity allows to calculate the relative dislocation density. The presence of hydrogen during cold rolling of palladium leads to an increase of dislocation density [3].

[1] M. Deutges et al., Scripta Mater.68 (2013) 71.
[2] R. Kirchheim, Acta Mater. 55 (2007) 5129.
[3] Y.Z. Chen et al., Scripta Mater. 68 (2013) 743.
[4] M. Deutges et al., Acta Mater. 82 (2015) 266.

MM 15.3 Mon 16:30 TC 006

The impact of the carbon content on hydrogen diffusion and its influence on hydrogen embrittlement for lab-cast bainitic Fe-C steels — •Emilie Van den Eeckhout, Tom Depover, and Kim Verbeken — Department of Materials Science and Engineering, Ghent University (UGent), Technologiepark 903, B-9052 Ghent, Belgium

The present work investigates hydrogen diffusion in lab-cast alloys in which a bainitic microstructure was introduced. The high diffusivity of hydrogen is a critical factor affecting hydrogen induced cracking since hydrogen is enabled to diffuse to highly stressed regions, leading to an accelerated failure. When hydrogen diffusion is impeded by introducing hydrogen traps, fracture is delayed and the susceptibility to hydrogen embrittlement is reduced.

The hydrogen diffusion coefficient is calculated using a permeation cell based on the Devanathan - Stachurski permeability cell. Decreasing the carbon content from 0.4 to 0.2 wt. % elevates the hydrogen diffusion, which can be attributed to less hydrogen traps of the latter bainitic steel. The impact of this higher diffusivity on the degree of embrittlement was evaluated by performing tensile tests on in-situ hydrogen charged samples at various cross-head displacement speeds. A correlation with melt extraction tests is made to demonstrate the combined effect of hydrogen content and hydrogen diffusion on hydrogen embrittlement. Additionally, the role of hydrogen diffusion is evaluated by calculating and visualizing, by in-depth fractography, the distance hydrogen can diffuse during a tensile test.

15 min. break

MM 15.4 Mon 17:00 TC 006

HYDROGEN EMBRITTLEMENT IN AEROSPACE MATERIALS — •Sathiskumar Jothi, Nick Croft, and Stephen GR Brown — Swansea University, Swansea, UK

Microstructures play a prominent role in aerospace components which are typically made of high toughness, corrosion resistant and high strength structural polycrystalline metallic materials such as nickel and nickel based super alloys. Nickel and nickel based super alloys are made up of complex microstructures which are susceptible to delayed failure caused by absorption of hydrogen produced either during fabrication in manufacturing process (i.e electrodeposition, welding etc*) or during operational use under environmental conditions. Several catastrophic failures have occurred in nickel and nickel based super alloys due to intergranular as well transgranular hydrogen embrittlement (HE) and hydrogen stress cracking (HSC) not only in aerospace industries but also in many other engineering sectors. HE depends on many factors including hydrogen diffusion and segregation, microstructural morphology and defects, stresses and texture morphological behaviour. Under EU FP7 *MultiHy* project, we employed multiscale technique to investigate the influence of these factors in hydrogen embrittlement

both computationally and experimentally. The studies provide insights on the influence of these factors and control it strategically to reduce the susceptibility of materials to hydrogen embrittlement

MM 15.5 Mon 17:15 TC 006

Investigation of Crack and Blister Formation Due to Hydrogen Loading in Iron — •Marie Tiegel[1], Annegret Lehmberg[1], May L. Martin[1], Martin Deutges[1], Christine Borchers[1], and Reiner Kirchheim[1,2] — [1]Institut für Materialphysik, University Göttingen, Germany — [2]International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan

Hydrogen-induced damage is a serious problem in various applications of metals and it is becoming more relevant as hydrogen is developed as a solution for energy storage. The mechanism of damage due to hydrogen is still ambiguous and requires further investigation. In this work, hydrogen- induced cracking (HIC) in high-purity iron was investigated. The samples were electrochemically loaded with hydrogen at different current densities. Hydrogen loading leads to cracks inside the bulk of iron, and the cracks near the surface create bubble-like defects on the surface above the cracks, called blisters. The microstructure of the cracks and blisters was investigated using SEM and TEM, including electron backscatter diffraction analysis. The surface curvature of the blisters consists of steps in the material, which is attributed to multiple individual crack advance events. TEM observations of the microstructure underneath the blister surfaces suggest that the formation of the blisters is due to the production of shear bands. Density measurements allow estimation of the pressure in the cracks, which is compareble to the yield stress of iron. In conclusion, the growth mechanism of blisters and cracks is due to a stress release following an increase of pressure in newly formed voids during hydrogen loading.

MM 15.6 Mon 17:30 TC 006

Hydride phase precipitation and growth in thin Nb-H films — •Vladimir Burlaka, Stefan Wagner, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Göttingen, Germany

In thin Me-H films below the critical thickness, hydrogen absorption and hydride precipitation are expected to be controlled by mechanical stress arising because of the interface matching between the film and the substrate as well as between the hydride precipitates and the surrounding host-matrix [1,2].

In the present study we experimentally address the effect of the film thickness on hydride precipitation and growth in Nb-H thin films of 15 - 40 nm. Hydrogen gas loading is performed for in-situ Scanning Tunneling Microscopy [1] and in-situ XRD measurements to study the hydride precipitates volume content, their lateral distribution and their mean lateral sizes. We found a strong change in the lateral distribution and the mean size at the critical film thickness, for similar pressures applied. It will be demonstrated that XRD pattern generally change when the film thickness is decreased below the critical thickness, making hydrides invisible [2]. But, STM images clearly verify the presence of hydrides even in the thin thickness range.

Financial support by the DFG via PU131/9 and PU131/12, as well as by the DESY/HASYLAB and the ESRF, Grenoble, are gratefully acknowledged.

[1] K. Nörthemann and A. Pundt, Phys. Rev. B 78 (2008) 014105. [2] V. Burlaka, S.Wagner and A. Pundt. accepted for publication in JALCOM.

MM 15.7 Mon 17:45 TC 006

Hydrogen loading kinetics of Mg Thin Films: effect of the driving force revisited — •Helmut Takahiro Uchida[1], Magnus Hamm[1], Stefan Wagner[1], Carsten Baehtz[2], Björgvin Hjörvarsson[3], and Astrid Pundt[1] — [1]Univ. Göttingen, IMP, Friedrich-Fund-Platz 1, 37077 Göttingen, Germany. — [2]Institute of Ion Beam Physics and Materials Research, HZDR, Germany — [3]Uppsala University, Dep. of Physics and Astronomy, Sweden.

Mg forms a dihydride with a high gravimetric hydrogen content of 7.6 wt% upon hydrogen absorption. This hydride is very stable and blocks hydrogen diffusion („Blocking effect“) [1,2]. This hinders the practical use of pure Mg for mobile applications, at low tempertures.

In this work, the impact of the driving force on the hydride formation kinetics in Mg films (200-2800 nm) is studied at room temperature, applying time-resolved *in-situ* XRD at different constant hydrogen gas pressures [3]. The evolution of inner stress is also monitored.

The hydrogen loading kinetics is found to strongly depend on the chemical potential. A heterogeneous hydride nucleation and growth model is suggested and evaluated by finite-element-calculatuion. The model allows qualitatively explaining the complex stress development, the different diffusion regimes and the blocking-layer thickness.

Financial support by the DFG via PU131/9 and PU131/10, as well as by the DESY/Hamburg and the ESRF/Grenoble are gratefully acknowledged. [1]J.Rydén *et al.*, *J. Less-Common Metals*, **152** (1989) 295. [2]H.T.Uchida *et al.*, *Script. Mater.*, **64** (2011) 935. [3]H.T.Uchida *et al.*, *Acta Mater.* (2014) (*Manuscript accepted*).

MM 16: Functional materials III: Sensors and Actuators

Time: Monday 15:45–17:45 Location: TC 010

MM 16.1 Mon 15:45 TC 010

Modified diamondoids for sensing applications — Frank Maier, Ganesh Sivaraman, Bibek Adhikari, and •Maria Fyta — Institute for Computational Physics, University of Stuttgart, Germany

Diamondoids are tiny diamond-like cages which are hydrogen terminated and can occur in various sizes and with a diverse type of modifications giving rise to novel bionanotechnological applications. In this work, based on quantum-mechanical calculations we study the effect of doping and functionalization of diamondoids on their structural characteristics and electronic properties. For this, we use different dopants and atomic groups and focus on the band-gap variations and the influence of the molecular orbitals in the case of the lower diamondoids, adamantane up to heptamantane. At a second step, we turn to the functionalized diamondoids and use these as probes to sense DNA molecules. Modified diamondoids can form hydrogen bonded complexes to DNA nucleobases tuning their electronic properties. Accordingly, we have observed that these small modified diamond-like cages are able to distinguish between small and large DNA nucleobases based on a difference up to 1 eV in the electronic band-gaps of the respective complexes. We discuss the possibility to sequence DNA through diamondoid-functionalized nanopores using quantum transport measurements. In the end, we discuss the theoretical stability of another class of diamondoids formed by nitrogen and boron instead of carbon and their relevance to nanotechnological applications.

MM 16.2 Mon 16:00 TC 010

Nanoporous gold as strain-sensing material — •Charlotte Stenner[1], Lihua Shao[1,2], Nadiia Mameka[3], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Beijing Institute of Nanoenergy and Nanoscience, Chinese Academy of Sciences, Beijing, China — [3]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Due to a large surface-to-volume ratio, nanoporous metals are predestined for exploiting their surface properties in schemes for novel functional materials. Here, we report an electrochemical sensor based on nanoporous gold (npg) for strain detection. Npg imbibed with electrolyte was inspected as a hybrid material, in which the metal acted as an electrode. Since the mechanical deformation of a planar gold electrode has a strong impact on its potential E [1], an applied strain is expected to cause potential variations that can be measured in npg.

In our experiments, macroscopic bulk samples of npg are cyclically strained in a dynamical mechanical analyzer (DMA). The material shows a robust and sensitive response of the potential to cyclic variation of strain. With higher strain amplitude and smaller pore size, the potential response is increased. Additionally, another strategy was employed, where a charge variation was measured at constant potential. Via this method the electrochemical signals were obtained in different potential regimes, as the double-layer and oxygen-adsorption region. [1] M. Smetanin, et al., Phys. Chem. Chem. Phys. 13 (2011) 17313

MM 16.3 Mon 16:15 TC 010

Shapeable magnetic sensorics — •Denys Makarov, Michael Melzer, Daniil Karnaushenko, Ingolf Mönch, Gungun Lin, and

Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Magnetic sensor elements are usually fabricated on rigid wafer supports and provided as IC-chip packages with defined shape and size. In order to explore advanced application fields imposed by the novel trend of printable, flexible, and stretchable high-speed electronics [1], functional magnetic elements have to feature the same compliant mechanical properties. Magnetic nanomembranes have the potential to fulfill these demanding requirements of being reshapeable on demand after their preparation. We developed the technology platform allowing us to fabricate high-performance shapeable, namely, flexible [2,3], printable [4] and even stretchable [5] magnetic sensorics. These novel magnetoelectronics can be printed onto a variety of materials including regular paper [4], rolled up into a compact tubular architectures for applications in fluidics [3], as well as be stretched up to 270% without degrading in performance. These unique mechanical properties enable applications of the novel magnetic sensing devices in medical diagnostics and functional implants, safety and health care monitoring, e-mobility, flexible and low-cost consumer electronics, soft robotics as well as artificial skins. [1] J. A. Rogers et al., Nature 477, 45 (2011). [2] Y.-F. Chen et al., Adv. Mater. 20, 3224 (2008). [3] G. Lin et al., Lab Chip 14, 4050 (2014). [4] D. Karnaushenko et al., Adv. Mater. 24, 4518 (2012). [5] M. Melzer et al., Nano Lett. 11, 2522 (2011).

MM 16.4 Mon 16:30 TC 010

Wearable magnetic field sensors for flexible electronics — •Gilbert Santiago Cañon Bermudez, Daniil Karnaushenko, Michael Melzer, Ingolf Mönch, Denys Makarov, and Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Dresden, Germany

The recent rapid advance and eagerness of portable consumer electronics stimulate the development of functional elements towards being lightweight, flexible, and even wearable[1]. Next generation flexible appliances aim to become fully autonomous and will require ultra-thin and flexible navigation modules, body tracking and relative position monitoring systems which frequently rely on Hall effect sensors. Unfortunately, conventional semiconductor-based Hall sensors are about 400 um thick and rigid, limiting their direct applicability in flexible electronics. To overcome this limitation of conventional technologies, we introduce a novel platform relying on the smart combination of inorganic Bismuth nanomembranes and polymeric foils, which allow us to fabricate highly flexible Hall effect sensorics[2]. Our experiments demonstrate that these flexible devices can be reliably bent or wrapped around the wrist to realize interactive devices for wearable electronics. Alternatively, thin and bendable Hall sensors are of great interest for the rapidly developing market of eMobility, where the performance of eMotor designs could be greatly enhanced.

[1] J. A. Rogers et al., Nature 2011, 477, 45.
[2] M. Melzer et al., Adv. Mat. (2014) in press.

15 min. break

MM 16.5 Mon 17:00 TC 010

Compact rolled-up antenna for implants applications — •Dmitriy D. Karnaushenko, Daniil Karnaushenko, Denys Makarov, and Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, Dresden

Smart implants were suggested as an efficient tool to monitor physiological processes in the human body, which is crucial especially after, e.g. chirurgical treatment. Compactness of the implants is highly desirable to minimize discomfort during and after implantation. If the length of the device is about 5 mm and diameter of less than 0.5 mm, it can be readily implanted using standard medical syringes. In this spirit, the rolled-up technology [1] was developed to realize multifunctional and compact 3D tubular devices by self-assembly starting from a planar layout. High-performance compact rolled-up active electronics, energy storage, magnetic field and fluidic sensors are already used to acquire and process the data [2,3]. However, the antenna element allowing the communication of the data to an external device, e.g. smartphone or personal computer, is missing. Here, we realized rolled-up helical antenna operating in the Industry-Scientific-Medical (ISM) radio band at 5.8 GHz. With a total length of 5.5 mm it is about 5 times smaller than the conventional dipole antenna. The transmission and receiving signals between rolled-up antennas and the communication between a rolled-up antenna and a smartphone is demonstrated highlighting its applicability for medical implant applications. [1] O. Schmidt et al., Nature 410, 168 (2001). [2] D. Grimm et al., Nano Lett. 13, 213 (2013). [3] I. Moench et al., ACS Nano 9, 7436 (2011).

MM 16.6 Mon 17:15 TC 010

Deformation characteristics and phase transitions in Fe_7Pd_3 thin films — •Alina J. Bischoff[1,2] and Stefan G. Mayr[1,2,3] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Translationszentrum für Regenerative Medizin, Leipzig — [3]Fakultät für Physik und Geowissenschaften, Universität Leipzig

Ferromagnetic shape memory alloys are a captivating class of smart functional materials and very promising candidates for miniaturized actuation devices featuring reversible strains of several percent due to the reorientation of twin variants in the martensite phase caused by an applied external magnetic field. In this context the ferromagnetic shape memory alloy Fe_7Pd_3 is of particular interest because of its high ductility, low brittleness, and corrosion resistance enabling the use of this alloy in micromedicine.

Within an in situ study, we explore the mechanical properties of martensite and austenite freestanding Fe_7Pd_3 thin films, while monitoring changes in the surface relief as measured by scanning electron microscopy. This allows to establish correlations between structural changes and mechanical respose.

MM 16.7 Mon 17:30 TC 010

Density functional investigations on the effect of Ni excess in binary Ni-Ti shape memory alloys — •Ingo Opahle[1], Jan Frenzel[2], André Wieczorek[2], Burkhard Maass[2], Gunther Eggeler[2], and Ralf Drautz[1] — [1]ICAMS, Ruhr-Universität Bochum, Bochum, Germany — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, Bochum, Germany

The martensite start temperature M_s of binary Ni-Ti shape memory alloys depends strongly on the alloy composition and decreases by about 100 K within 1 at.% of excess Ni. We present density functional calculations for binary Ni-Ti alloys close to the stoichiometric composition. In agreement with experimental results it is shown that the heat of transformation ΔH decreases as the Ni concentration increases, which in turn results in a lower martensite start temperature. The strong decrease of ΔH is caused by a stabilization of the B2 austenite phase by structural relaxations around Ni antisite atoms together with a gradual destabilization of the B19' martensite phase. In contrast, contributions from the valence electron count or magnetism are shown to be unable to explain the experimentally observed changes in M_s.

MM 17: Postersession I

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

MM 17.1 Mon 18:00 Poster E

Microstructural characterization of hydrogen induced cracking in TRIP-assisted steels by EBSD — •Aurélie Laureys, Tom Depover, Roumen Petrov, and Kim Verbeken — Department of Materials Science and Engineering, Ghent University (UGent), Technologieparkt 903, B-9052 Ghent, Belgium

The present work evaluates hydrogen induced cracking in a TRIP-assisted steel with a complex multiphase microstructure, containing ferrite, bainite and retained austenite. When deformed, the retained austenite transforms to martensite and each structural constituent demonstrates a different behavior in the presence of hydrogen. The goal of this work is to understand the response of the hydrogen saturated multiphase structure to a mechanical load. Tensile tests on notched samples combined with in-situ electrochemical hydrogen charging were performed. The tests were interrupted at a stress just after reaching the tensile strength, since hydrogen induced cracks were found to form after reaching the tensile strength. Such interrupted tests allowed to study hydrogen induced crack initiation and propagation in the material. The microstructure of the samples was characterized by means of scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD). A correlation was found between the occurrence of martensite, which is known to be very susceptible to hydrogen embrittlement, and the initiation of hydrogen induced cracks. The latter were located on the surface in specific high-stressed regions, which were induced due to the presence of the notch.

MM 17.2 Mon 18:00 Poster E

Growth Process of Hydrogen Induced Structures on Gd Films and Islands Observed by STM — •Sara Wanjelik, Samuel Königshofen, and Mathias Getzlaff — Institute for Applied Physics, University of Düsseldorf

Hydrogen in metals as an area of research has been of great interest for the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamental point of view. But only few investigations are carried out by imaging techniques with a lateral resolution on the nm-scale. Even less works deal with the initial stage of hydride formation.

Here we present STM measurements on thin Gadolinium films and islands grown on a W(110) surface under ultra high vacuum conditions. On Gd-films two kind of hydrogen induced modifications can be observed: Hydrides and small disc-like islands with a diameter of a few nm and a height of one atomic step. The discs form chains with clearly preferred directions. A triangular shaped structure is observed together with the discs. The growth process of these modifications were studied in detail. Electronic differences of the described structures were investigated by maps of differential conductivity.

Contrary to films islands can be penetrated by hydrogen from the side walls. Therefore, the hydride formation should start from the edges. Another difference to films is that not only a vertical expansion, due to the larger volume of the hydride, is possible but also a lateral.

MM 17.3 Mon 18:00 Poster E

Kinetics of Hydrogen uptake in epitaxial thin films of Niobium — •Niklas Teichmann, Vladimir Burlaka, Stefan Wagner, and Astrid Pundt — Univ. Göttingen, IMP, Friedrich- Hund-Platz 1, 37077 Göttingen, Germany.

Hydrogen located in interstitial lattice sites changes physical properties of the host metal, such as the resistivity or the lattice parameter.[1,2] Even though both physical properties are not linearly coupled to the hydrogen content, strong changes occur upon phase transitions. Therefore, they can be used to determine the concentration change and the onset of phase transition in thin films. In this paper we report on in-situ studies on the kinetics of the hydrogen uptake in thin Nb films (8 nm - 40 nm) with different Pd capping layers (0,2 nm - 20 nm). All experiments are performed without breaking the UHV conditions. Hydrogen is loaded step-wise from the gas-phase. It will be shown that even down to a Palladium capping layer thickness of 2 nm the kinetics of Hydrogen uptake is fast. It is dramatically reduced below that thickness. This effect is attributed to an island-like Pd-layer morphology that arises for the thinnest capping layer thicknesses. Also, the unloading kinetics is reduced when island-like capping layers are used.

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

[1] A. Pundt, R. Kirchheim, Ann. Rev. Mater. Sci. 2006

[2] K. Nörthemann, & A. Pundt, (2008). Coherent-to-semi-coherent transition of precipitates in niobium-hydrogen thin films. Physical Review B, 78(1), 014105.

MM 17.4 Mon 18:00 Poster E

H-Diffusion in Mg-Fe11at% Alloys — •Magnus Hamm, Helmut Uchida, and Astrid Pundt — Universität Göttingen, IMP, Friedrich-Hund-Platz 1, 37077 Göttingen

In the last decade Magnesium (Mg) has attracted much interest as a storage material for hydrogen. The reasons are its high reversible hydrogen capacity of up to 7,6 wt% and its high volumetric capacity of 110 kg/m^3 [1]. However the slow hydrogen (de)absorbtion kinetics of Mg and its high desorption temperature provide a significant barrier to Magnesium's commercial use [2]. Iron (Fe) is known to improve the hydrogen uptake rate in Mg [3]. To study the influence of Fe on the kinetics of Mg, 500 nm Mg-Fe alloy films were prepared by Argon-ion-beam sputtering and loaded from the gas phase. The hydrogen uptake was studied in-situ with synchrotron radiation at DESY/Hamburg and ESRF/Grenoble. It will be demonstrated that the diffusion constant, while lower than in pure Magnesium, was orders of magnitude above the recorded diffusion constant of MgH2. In addition, with the used parameters full loading of the Mg-Fe samples is possible without any sign of a blocking layer. This differs strongly to what was found by H. Uchida et al.[4] on pure Mg films of similar thickness.

Beamtime provided at the DESY/Hamburg and the ESRF/Grenoble is gratefully acknowledged. This project is financially supported by the DFG via Project PU131/9-1 and PU131/10-1.

[1] Dornheim, R. et al., Scr. Mat. 56:10 (2007) [2] Bogdanović, B. et al., J. Alloys Compd. 282:1-2 (1999) [3] Holtz, R.L. and Imam, M.A., J. Mater. Sci. 34:11 (1999) [4] Uchida, H. et al., Acta Mat., accepted

MM 17.5 Mon 18:00 Poster E

Hydrogenography-Study of thin Vanadium-Hydrogen films — •Anshu Tyagi, Jantje Schommartz, and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In this work, thin Vanadium films of 10 nm - 30 nm thickness, sputter deposited on transparent Glass substrates are examined. These samples are electrochemically loaded with hydrogen while simultaneous measurements of the transmission and reflection are done with a Light microscope. Electrochemical hydrogenography offers the possibility to study the local and the global hydrogen concentration within a defined area of the film and hence gives information on the lateral hydrogen distribution on a micrometer scale. Also the role of nucleation and growth in the hydrogenation of films is analyzed by using a mask technique during film deposition. In-situ Scanning Probe Microscopy studies are additionally performed. The role of the local detachment on the local hydride nucleation is examined by repeated loading experiments.

[1] J. Kürschner, S. Wagner, A. Pundt, Journal of Alloys and Compounds 593 (2014) 87-92. [2] L. Mooij, B. Dam, Phys. Chem. Chem. Phys. 15 (2012) 2782-2792. [3] J.L. Schommartz, Bachelor Thesis, University of Göttingen, (2014).

Financial support by the DFG via DFG-PU131/9-1 is gratefully acknowledged.

MM 17.6 Mon 18:00 Poster E

Optimized Pd/TiO_2 interfaces for high resolution TEM-EELS in H_2 atmosphere — •Marian Bongers, Carsten Nowak, and Astrid Pundt — Institut für Materialphysik, Georg-August-Universität Göttingen, Germany

Redox reactions on supported metal catalysts exhibit high turnover rates [1, 2]. The used support strongly influences the turnover rate and, therefore, the metal/support interface is expected to be a very important parameter. Atomic resolution STEM and EELS allow to investigate the electronic states at Pd/TiO_2 interfaces, which are expected

to change under hydrogen atmosphere as suggested by Kobayashi et al. [3], thus eventually giving insight into the enhanced turnover rates.

Here we report on the preparation of optimized Pd/TiO_2 double layers. The layers were deposited by magnetron sputtering. XRD and texture measurements reveal epitaxial growth of a strained Pd-film on a single crystalline TiO_2 film.

EELS investigations on the electronic states in the vicinity of the Pd/TiO_2 interface are presented. Changes of the electronic states related to the presence of hydrogen are discussed. Additional EELS measurements on the oxygen edge show a strong dependency of the signal/noise ratio on the lamella thickness.

[1] D.C. Grenoble, M.M. Estadt, Journal of Catalysis 67 (1981) 90; [2] M. Bowker et al., Surface Science 497 (2002) 155; [3] H. Kobayashi et al., Surface Science 304 (1994) 393

Financial support by the DFG via SFB1073-C06 and DFG-PU131/9-1 is gratefully acknowledged.

MM 17.7 Mon 18:00 Poster E

Hydrogen-induced stress in ultrathin Nb-Fe Films — •Philipp Klose[1], Magnus Hamm[1], Helmut Klein[2], and Astrid Pundt[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Geowissenschaftliches Zentrum Göttingen, Goldschmidtstr. 1-3, 37077 Göttingen, Germany

Hydrogen which is located in interstitial lattice sites, is an origin for compressive mechanical stresses in thin films[1,2,3]. For low hydrogen concentrations, the in-plane film stress increases linearly on the hydrogen content.[3] Above a hydrogen-related yield stress the films deform plastically[4]. In this study, the hydrogen-induced stress development in niobium-iron (Nb_{90}-Fe_{10}) films is examined. The focus is on the thickness dependency of the stress development and the determination of the yield stress in these films.

The films of 3 nm - 40 nm were prepared by argon-cathode beam sputtering. They were studied by XRR-measurements to determine the exact film thickness. For selected samples the texture of the Nb-Fe films was determined by XRD to evaluate their epitaxial growth. Hydrogen loading was performed from the electrolyte using constant current conditions. The hydrogen concentration was determined via Faraday's law. The hydrogen-related yield stress is found to be strongly thickness dependent, in the thickness range studied.

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MM 17.8 Mon 18:00 Poster E

Correlation between thermodynamic and mechanical properties in binary bcc alloys — •Sandra Hoppe, Sascha B. Maisel, and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

When aiming at high-performance tailored metal alloys, it is crucial to understand basic material properties and their relation. Modern computer simulation methods like the cluster expansion with input from density functional theory calculations make the whole configurational space accessible. This way, also metastable structures may be considered, which are experimentally difficult to obtain. 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. We investigated this relation between the formation enthalpy and the elastic constants c_{44} and c_{11} for several binary body-centered cubic (bcc) phases with alloying elements with bcc, fcc or hexagonal close-packed (hcp) equilibrium lattices and at different concentration regimes to understand the basic mechanisms behind this phenomenon. Interestingly, some alloys show similar trends to the fcc alloys, while Ta-W exhibits and anomalous behavior of c_{44} at the central concentration regime: Energetically favorable structures are mechanically less stable than those further away from the ground-state line.

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MM 17.9 Mon 18:00 Poster E

A density functional theory study on elastic and thermodynamic characteristics of Al_5Fe_2 — •René Wirnata, Lilit Amirkhanyan, and Jens Kortus — Institute of Theoretical Physics, TU Freiberg, Deutschland

Based on density functional theory calculations, the η-Al-Fe binary phase of the quasi-crystal Al_5Fe_2 was studied. Since these calculations require an ideal crystal, an approximant for the starting structure [1], which contains channels of partially occupied sites, had to be constructed. Thermodynamic properties like the heat capacity at constant pressure and volume or the thermal expansion coefficient were calculated using the quasi-harmonic approximation. In addition, the elastic properties of this system as well as the magnetic Stoner criterion were analyzed.

For the heat capacity, the theoretical results could be compared with three experimental data sets [2,3,4]. In case the electronic contribution was incorporated, excellent agreement with two of these studies can be reported.

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[4] T. Zienert, TU Freiberg - Institute of Material Sciences

MM 17.10 Mon 18:00 Poster E

On the atomistic diffusion processes in Cu65Zr35 metallic glass by molecular dynamics simulations — •Pablo Palomino[1], Giorgos Almyras[1], Dimitris Papageorgiou[2], and Giorgos Evangelakis[1] — [1]Department of Physics, University of Ioannina, Ioannina 45110 Greece — [2]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece

Metallic Glasses (MG) are characterized by lack of long range order and periodicity. This particularity affects seriously most of their properties, including diffusion. Despite the serious research efforts in the last decades, both experimentally and theoretically, aiming in revealing the microscopic aspects of diffusion in MGs, several questions remain still open mainly referring to the diffusion mechanisms, the empty space required for a diffusion event to occur, the energetic requirements or the driving force, e.t.c.. In the present study we performed MD simulations on a well known model MG (Cu-Zr) focusing on the microscopic aspects of diffusion in both the supercooled and below the glass transition temperature regions. It came out that diffusion takes place by means of short distance atomic displacements, which become consecutive at high temperatures and are activated by the collective vibrations of neighboring atoms. Several relevant to diffusion processes quantities were evaluated, quantified and compared with available data in the literature in the whole temperature region studied. We think that the present results could be used to enlighten phenomena related to slow diffusion like aging or creep relaxation.

MM 17.11 Mon 18:00 Poster E

In-situ Delithiation of $LiMn_2O_4$ by Laser Assisted Atom Probe Tomography — •Jonas Arlt, Björn Pfeiffer, Johannes Maier, and Carsten Nowak — Georg-August-Universität Göttingen, Institut für Materialphysik, 37077 Göttingen, Germany

Manganese dioxides have been extensively studied as cathodematerial in rechargeable Li-ion batteries. Understanding ionic conduction and energy conversion processes in the cathodematerial is crucial for the optimization of Li-ion batteries. Current experimental data is usually obtained with methods characterizing transport on a macroscopic scale, but particularly for phase separating materials transport is expected to be strongly localized. To overcome this, atom probe tomography (APT) and related techniques have been further developed to obtain local information on the chemical composition and ionic transport with sub nm resolution [1, 2].

Here, we present Laser-APT studies on $LiMn_2O_4$. Modifying the experimental conditions during the measurement allows in-situ studies of the delithiation process, revealing insights into ionic transport mechanisms. Using a focused ion beam, nanoscopic $LiMn_2O_4$ tips were prepared. Sample morphology and crystal structure were determined by transmission electron microscopy. The influence of the applied electric field, temperature and laser parameters on the delithiation process will be discussed.

References

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MM 17.12 Mon 18:00 Poster E

Probing magnetic phase transitions in Heusler-alloys and Magnetite using EMCD — •Walid Hetaba[1,2], Stefan Löffler[1], Michael Stöger-Pollach[1], Andreas Hütten[3], Gareth Parkinson[4], Marc-Georg Willinger[2], and Robert Schlögl[2] — [1]USTEM, Vienna University of Technology, Austria — [2]Department of Inorganic Chemistry, Fritz Haber Institute of the MPG, Berlin, Germany — [3]Thin Films and Physics of Nanostructures, Department of Physics, Bielefeld University, Germany — [4]Institute of

Applied Physics, Vienna University of Technology, Austria

Energy-loss magnetic chiral dichroism (EMCD) is a versatile technique to investigate magnetic properties on the nanoscale. Heusler-alloys and Magnetite are promising systems in the field of spintronics. Furthermore, multilayer Heusler systems are used for ferroic cooling applications. These alloys show an austenitic-martensitic phase transition, where the transition temperature depends on the actual elemental composition. Magnetite shows a Verwey transition at about 120 K. In this work, we perform in-situ EMCD measurements to investigate the changes of the magnetic properties at different temperatures. The experimental results are found to be in very good agreement with simulations. These simulations are crucial as dynamical diffraction affects the intensity of the measured EMCD signal, bringing the sample thickness into the game. By combining theory and experiments, this study paves the way for tailoring the magnetic phase transition of materials for the use in spintronics. The Austrian Science Fund is acknowledged for financial support under grant numbers F4501-N16 and I543-N20.

MM 17.13 Mon 18:00 Poster E

Resolution analysis of Transmission Kikuchi Diffraction (TKD) patterns in SEM — •Dennis Langenkämper, Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Since the first commercial systems appeared in the early 1990s, electron back-scatter diffraction (EBSD) has grown into one of the most common techniques to characterize the microstructure of crystalline samples. Due to its ease and vast range of applicability to materials in the submicrometer grain size range, EBSD is a widely spread method to analyze deformation structures and mixtures of phases.

Current research focuses on nanoscaled materials, which may show drastic changes in properties with often superior results. Thus, there is a strong need to enhance the spatial resolution of EBSD. Transmission Kikuchi Diffraction (TKD) is a suitable method to overcome limits of EBSD by using thin samples transparent to the electron beam.

The present work focuses on the resolution limits, using a conventional EBSD detector (EDAX) and a custom-build TKD sample holder to study the influence of experimental conditions (sample thickness, sample material) on the resolution limit of TKD.

MM 17.14 Mon 18:00 Poster E

Non-isothermal crystallization kinetics of metallic glass by differential fast scanning calorimetry — •Bin Yang[1], Yulai Gao[2], and Christoph Schick[1] — [1]AG Polymer Physics, Institute of Physics, University of Rostock, Germany — [2]School of Materials Science and Engineering, Shanghai University, Shanghai, P.R. China

The thermal stability and the kinetic fragility of Al86Ni6Y4.5Co2La1.5 (%wt.) metallic glass were investigated by ultra-fast non-isothermal thermal analysis. The differential fast scanning calorimeter (DFSC) traces revealed that the material undergoes a three-stage crystallization for heating rates ranged from 5 to 40,000 K/s. Combining DSC and DFSC, the kinetics of the glass transition and crystallization of Al86Ni6Y4.5Co2La1.5 metallic glass was investigated. The kissinger plot can express the temperature dependence of growth rate of this metallic glass. Furthermore, the kinetic fragility for Al86Ni6Y4.5Co2La1.5 metallic glasses is evaluated. Depending on the fragility index, this metallic glass is a liquid of very high fragility, similar to several organics.

MM 17.15 Mon 18:00 Poster E

Low frequency acoustic measurements on the metallic glass $Zr_{46.8}Ti_{8.2}Cu_{7.5}Ni_{10}Be_{27.5}$ — Sebastian Craft, •Arnold Seiler, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

The properties of amorphous solids at low temperatures are well known to be dominated by atomic two-level tunneling systems (TS). While the standard tunneling model successfully describes thermodynamic properties of insulating glasses it fails to predict the elastic properties of metallic glasses. To investigate the role of conduction electrons on the density of states and the dynamics of TS vibrating reed experiments are performed. In superconducting glasses the interaction can be switched on and off by means of a magnetic field which suppresses superconductivity and therefore enables electrons to interact with TS. Here we present measurements of the internal friction and the sound velocity of the splat cooled superconducting metallic glass $Zr_{46.8}Ti_{8.2}Cu_{7.5}Ni_{10}Be_{27.5}$ measured at frequencies between 600 Hz and 14 kHz and temperatures from 10 mK to room temperature. Within these experiments we used an improved sample geometry to reduce clamping losses and to excite different modes at various frequencies.

MM 17.16 Mon 18:00 Poster E

Impact of minor-alloying on the mechanical properties of Pd-based bulk metallic glasses — •Niklas Olschewski, Niklas Nollmann, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Metallic glasses offer unique properties such as high strength, extended elasticity, high wear and corrosion resistance. However, the limited ductility and especially the immediate catastrophic failure in tension once the elastic limit is reached are major obstacles to applications as structural materials. This behavior has led to substantial effort towards understanding and improving the accommodation of plastic deformation in metallic glasses, including the design of composites consisting of glassy material surrounded by ductile crystallites. Our work has focused on the improvement of the ductility of bulk metallic glasses by adding minor alloying elements. In particular the impact of adding slight amounts of cobalt or iron (0.2 - 4 wt.%) to the well-known bulk glass-former $Pd_{40}Ni_{40}P_{20}$ on the mechanical properties has been studied.

The samples were produced by copper mold casting and their mechanical behavior was tested in compression and three-point bending tests. Further investigations (e.g. DSC, XRD, ultrasonic measurements, SEM) have been conducted to characterize the alloys' properties. The obtained results are discussed.

MM 17.17 Mon 18:00 Poster E

Processing and characterization of a deformed ZrCu metallic glass with tunable content of nanocrystallites — •Marius Gerlitz, Jonas Bünz, Martin Peterlechner, and Gerhard Wilde — Westfälische Wilhelms-Universität, Münster, Deutschland

The deformation mechanisms of metallic glasses are in focus of current research. In the present work, a ZrCu-based glass with a nominal composition of $Zr_{53.8}Cu_{31.6}Ag_{7.0}Al_{7.6}$ (at. %) was processed by arc melting and subsequent melt-spinning. Upon heating, controlled growth of crystallites occurs at well-chosen temperatures and times. A study is carried out by systematically varying the annealing parameters of the as-produced amorphous sample using differential scanning calorimetry (DSC). Determination of the crystallization kinetics leads to the ability to tailor the volume fraction of nanocrystallites embedded in the amorphous matrix. The obtained nanocrystallites are observed by transmission electron microscopy (TEM). Subsequently to an annealing treatment to obtain partial crystallization, the material is deformed by cold rolling using a two-high rolling mill. This method leads to the generation of shear bands. TEM analysis was carried out to analyze shear bands and their interaction with nanocrystallites. The results are discussed with respect of the impact of nanocrystalline precipitates on the propagation of shear bands in a metallic glass.

MM 17.18 Mon 18:00 Poster E

Liquid Metallic Hydrogen and Solar Physics — •Alexander Unzicker — Pestalozzi-Gymnasium München

The metallic state of hydrogen, postulated by Wigner and Huntigton in 1935, presents both experimental and theoretical challenges and is a topical research field in condensed matter physics. In particluar, it has been hypothesized that liquid metallic hydrogen may be metastable at normal conditions. Focussing on the unique character of hydrogen as 'zeroth' alkali metal, the ranges of possible pressures and temperatures are discussed.

The existence of a metastable state would have profound consequences for understanding of the sun, since a series of observations supports the idea that the sun's surface is liquid. These arguments have been advanced in much detail by Pierre-Marie Robitaille, a renowned radiologist, but have received little attention in the solar physics commmunity so far.

The talk also tries to enhance the communication across different fields of physics that is sometimes necessary when a long established paradigm - in this case the standard solar model - is in trouble. Disussions are particlularly welcome.

MM 17.19 Mon 18:00 Poster E

Thermally induced hydrogen desorption of metal-borohydrides — Christoph J. Sahle[1], Simon Kujawski[2], Arndt Remhof[3], Yigang Yan[3], Nick Stadie[3], Kolja Mende[2], Ali Al-Zein[1], Simo Huotari[4], Metin Tolan[2], and •Christian Sternemann[2] — [1]European Synchrotron Radiation Facility, Greno-

ble, France — [2]Fakultät Physik / DELTA, Technische Universität Dortmund, Dortmund, Germany — [3]Empa, Hydrogen and Energy, Dübendorf, Switzerland — [4]Department of Physics, University of Helsinki, Helsinki, Finland

Complex lightweight hydrides are candidates for efficient reversible hydrogen storage. During dehydrogenation the hydrides decompose into both crystalline and amorphous phases where latter are often difficult to detect. We use x-ray Raman scattering, a bulk sensitive probe of soft x-ray absorption edges, to measure e.g. boron K- and magnesium L-edges both ex-situ and in-situ during decomposition. To clarify possible decomposition pathways, spectra of reference samples are employed to fingerprint intermediate phases via principal component analysis. Results for magnesium and calcium borohydrides will be discussed with focus on the formation of closo-borane species, which could act as a boron sink and hinder cycling.

MM 17.20 Mon 18:00 Poster E

Potential-strain coupling during hydrogen electroabsorption — •Shan Shi[1], Tobias Kitzler[1], Qibo Deng[2], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Insitut für Werkstoffforschung, Werkstoffmechanik — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie

The recent past has seen an increasing interest in the impact of mechanical deformation on the electrode processes. The effect is measured by the potential-strain coupling coefficient (ς) which quantifies the variation of the electrode potential, with tangential strain. In this study, we use dynamic electro-chemo-mechanical analysis (DECMA) to determine the potential-strain coupling during hydrogen electroabsorption into a Palladium (Pd) thin film. The samples are prepared by DC magnetron sputtering of a nanometer thick Pd film, which contains many grain boundaries, on a polyimide substrate. We monitor the electrochemical behaviour of the Pd thin film in aqueous electrolytes during imposing periodical elastic strain on the sample. Additionally, another customised in-situ electrochemical cell enables us to determine microstructural information of the Pd film such as the lattice parameter by in-situ X-ray diffraction. By combining the results, the question how the mechanical strain affects the storage of light interstitials (H) in Pd and the kinetics of the adsorption or dissolution at the electrode surface and the absorption in the grain boundaries and the bulk will be explored.

MM 17.21 Mon 18:00 Poster E

In-situ TEM of phase transitions in TiNi based shape memory alloys — •Timo Wuttke and Cynthia Ann Volkert — Institute of Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Shape memory alloys (SMA) are known for their ability to recover plastic deformation upon heating and thus may be used for applications such as actuation in a wide range of industry, science and medical related fields.

The key mechanism responsible for this behavior is a reversible diffusionless solid-state phase transition between a highly twinned martensitic state and an untwinned austenitic phase of higher crystal symmetry.

We studied the martensitic phase transition of TiNi and TiNiCu alloys utilizing in-situ TEM techniques. Both commercially available wires and samples prepared with vacuum arc melting were used. All samples were annealed at 600°C for 1,5h and water quenched to ensure that the phase transition takes place between RT and 100°C thus making it easily accessible in the TEM.

The movement of the austenite-martensite reaction front can be directly observed and manipulated by applying temperature gradients to the TEM lamella. This allows us to study the phase transformation with high spatial resolution. Atomic level information obtained at the moving phase boundary using HRTEM will be discussed.

MM 17.22 Mon 18:00 Poster E

Gas sensors based on metal oxides deposited on AAO for the detection of carbon monoxide — •Jonas Lübke, Stefan Ostendorp, Nina Winkler, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Germany

Carbon monoxide is a colourless, odourless, flavourless and non-irritant gas produced from partial oxidation of carbon-containing compounds. If inhaled, it connects to the central iron atom of haemoglobin and therefore prohibits oxygen transport in blood, which leads to death by choking. Therefore sensitive and reliable detection is of great interest. Carbon monoxide acts reductive on most oxidized semi-conductors (SC's), leading to increased or decreased resistance, depending on whether they are n- or p-type SC's. Former work has shown successful detection of CO with metal oxide semi-conductors (MO-SC) on glass substrates. To increase the detecting surface and the inspected volume, use of "Anodic Aluminum Oxide" (AAO)-membranes as substrate seems to be promising. To this end, metal oxides were deposited on AAO via atomic layer deposition (ALD). The gas sensor set-up is brought into a temperature-controlled vacuum chamber to provide the required activation energy for chemisorption of CO in a defined gas environment. A well-defined amount of air is introduced to the chamber and then a well-defined amount of CO. The current through the sample/gas sensor is measured via a four probe measurement. The effect of modifications of the membranes and oxide films concerning the resultant gas sensing properties was examined.

MM 17.23 Mon 18:00 Poster E

A novel kind of solid state thin film battery — •Yaser Hamedi Jouybari and Frank Berkemeier — Institute of Material Physics, Westfälische Wilhelms-Universität Münster, Münster, Germany

Thin film lithium batteries (TFBs) are regarded as next Generation of energy storage devices for highly specialized applications. In our work we investigate a novel kind of TFB that consists of high-performance active materials. In particular, we are using thin films of LiFePO4 as cathode, LiPON as solid electrolyte, and silicon as anode. All materials are prepared by sputtering, to achieve a well-defined thickness and uniformity of the layers. To investigate the electrochemical behavior of these TFBs, the overall battery cells, as well as the individual battery components, are studied by transmission electron microscopy, atomic force microscopy, cyclic voltammetry, chronopotentiometry, and impedance spectroscopy.

In our studies it turned out that the transport across the interfaces between the electrolyte and the electrodes is most critical to TFB performance. This transport is heavily affected by some disturbing phenomena such as unwanted reaction layers, roughness of the solid electrolyte, and its degradation during subsequent deposition processes. To increase the interface quality, all of these phenomena need to be minimized and controlled by deposition parameters. Hence, in our work we report on the dependence of the TFBs performance on the deposition parameters, with particular focus on the properties of the LiPON under different deposition conditions.

MM 17.24 Mon 18:00 Poster E

Atomistic simulations of materials relevant for nuclear waste management — •Yaqi Ji, George Beridze, Yan Li, and Piotr Kowalski — Institute of Energy and Climate Research: IEK-6 Nuclear Waste Management and Reactor Safety, Forschungszentrum Jülich, Jülich, Germany

Safe management of nuclear waste represents a challenge for nuclear energy utilizing countries. Thus, a significant research effort has been devoted to investigate the potential solid nuclear waste forms in which radionuclides could be immobilized under repository conditions and stored for even geological times. The goal of such research is the full characterization of properties of these materials upon incorporation of actinides into their crystalline structures. One challenge related to the atomistic modelling of these strongly correlated materials is the proper description of their electronic structure. In that aspect we present our results on benchmarking the DFT+U method for derivation of the thermochemical properties of actinide-bearing molecular compounds and solids [1] and its application to the computer-aided characterization of the potential disposal waste form materials such as monazite-type ceramics ($Ln\mathrm{PO}_4$) and pyrochlore [2,3]. In particular we will present results of investigation of the thermodynamic stability of these ceramics [3] under potential repository conditions and simulations of radiation damage effects in these materials.

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MM 17.25 Mon 18:00 Poster E

3D nanofabrication of subsurface structures inside photosensitive glass with fs laser — •Tobias Milde[1], Ulrike Brokmann[2], Edda Rädlein[2], and Klaus Liefeith[1] — [1]Department of Biomaterials, Institute for Bioprocessing and Analytical Measurement Techniques Heiligenstadt — [2]Group of Inorganic-Nonmetallic Materials, Department of Mechanical Engineering, Technische Universität Ilme-

nau

The development of miniaturized structures on or below the surface of glass is an issue of present research. Femtosecond-laser-radiation combined with the two photon process is a promising approach to push the written structures towards the nanometer scale. Here we used the photosensitive glass FS21 with its three step photoform process (irradiation, annealing, HF-etching). For the irradiation we used a TiSa oscillator only. These structures and steps are developed to realize a distinct miniaturization of glass components and to improve biocompatibility for specific cells. This structured glass is interesting for microfluidic and lab-on-a-chip devices. Here we present new scientific findings to material characterization and the photoform process.

MM 17.26 Mon 18:00 Poster E

Phase equilibria and interfacial properties of a curved liquid-solid interface — •Muhammad Ajmal Choudhary[1], Julia Kundin[1], Martin Oettel[2], and Heike Emmerich[1] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth — [2]Institut für Angewandte Physik, Universität Tübingen, D-72076 Tübingen

The phase field crystal (PFC) technique is a novel approach for modeling crystal growth phenomena with atomistic resolution on mesoscopic time scales. We use a 2D PFC model for a binary system based on Elder et al. [Phy. Rev. B 75, 064107 (2007)] to establish a precise assessment of the nucleation mechanisms beyond classical nucleation theory. More specifically, we investigate the equilibrium properties of a curved liquid-solid interface as well as the nucleation barriers. We propose the method of determining interfacial energies for a curved liquid-solid interface in a finite system by stabilizing the circular solid crystal of various radii in the surrounding liquid phase and liquid droplets of various radii in the corresponding solid phase. We suggest a phenomenological expression to describe the dependence of the extracted interface tension on the nucleus radius r for the liquid-solid system. The numerical PFC results show that this dependency can not be fully described by the non-classical Tolman formula. Moreover, we also derived the free energy barriers for the nucleation and compared the results with predictions based on classical nucleation theory.

MM 17.27 Mon 18:00 Poster E

Atom probe tomography studies of the effects of industrial heat treatment on the precipitation kinetics on aluminum alloy 2195 — •Muna Khushaim[1], Judith Seibert[2], Ferdinand Haider[2], and Talaat Al-Kassab[3] — [1]Physical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia. — [2]University Augsburg, Inst. f. Physics, D -86159 Augsburg, Germany. — [3]D-37077, Göttingen, Germany.

Aluminum lithium alloys are of great interest for commercial, military and aerospace applications. These alloys possess high strength, light weight, low density and good mechanical properties.The superior mechanical properties of this alloy is owing to the presence of different intermetallic phases such as T_1 (Al_2CuLi), $\theta^{'}$ (Al_2Cu), $\delta^{'}$ (Al_3Li) and $\beta^{'}$ (Al_3Zr).The objective of this work is to provide insight into the relationship between precipitation sequences, mechanical properties and the preformed heat treatment conditions. Aluminum alloy 2195 was selected as a model system in the present study. Different industrial heat treatments such as: T8 temper, T4 temper and T6 temper were applied on the alloy. Utilizing laser assisted wide angle tomographic atom probe (LAWATAP) and local electrode atom probe (LEAP) allowed the investigation of precipitation kinetics and phase transformation phenomena. Data will be presented will highlighting the role of the industrial heat treatment on the developing of the microstructure, along with an in depth study of distribution of different alloying elements in the strengthening phases.

MM 17.28 Mon 18:00 Poster E

Microstructure and electrical characterization of commercial Na-β-Alumina — •Wolfram Münchgesang[1], Torsten Schucknecht[2], Barbara Abendroth[1], Tilmann Leisegang[1,3], David Rafaja[2], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Freiberg, Germany — [2]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Freiberg, Germany — [3]Fraunhofer-Technologiezentrum Halbleitermaterialien THM, Freiberg, Germany

Na-β-Alumina (NaBA) is a well-known and commercially available solid electrolyte (SE) for high-temperature Na-S-accumulators (NSA). Under conditions of standard working temperatures of around 300 °C NaBA is stable, electrically insulating and ion-conducting.

These properties make NaBA also interesting for low-temperature NSA, as an alternative separator and as a reference for SE. The challenge for the transfer from a high- to a low-temperature working SE is to compensate the strong decreased ion-conductance by a decreased thickness, without reducing its stability and insulating properties. In this regard, the microstructure of NaBA and its influence on the conductivity has to be worked out and controlled during preparation.

We will present and discus results on multiscale investigation of commercial NaBA exhibiting a complex defect structure. This involves the analysis of the chemical and phase distribution as well as the microstructure and their influence on the conductivity.

This work was financed by der Federal Ministry for Economic Affairs and Energy within the project BaSta (0325563D).

MM 17.29 Mon 18:00 Poster E

Pressure-induced spin transition of Fe^{2+} in siderite $FeCO_3$ studied by x-ray Raman scattering — •Christopher Weis[1], Christian Sternemann[1], Max Wilke[2], Valerio Cerantola[3], Christoph J. Sahle[4], Georg Spiekermann[5], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Helmholtz-Zentrum Potsdam, German Research Centre for Geoscience (GFZ), 14473 — [3]Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany — [4]ESRF, 38043 Grenoble Cedex 9, France — [5]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Pressure-induced electronic and/or structural transitions of iron bearing compounds at conditions of the inner earth fundamentally affect the material's properties, e.g. sound velocitiy and density. Siderite ($FeCO_3$) forms a complete solid solution with magnesite ($MgCO_3$). Owing to the low solubility of carbon in the mantle it is a candidate for carbon storage and a key mineral to understand the Earth's carbon cycle. Lavina et al. [1] applied high-pressure x-ray diffraction to siderite and found a high-spin to low-spin transition to occur at 43-49 GPa with a sharp volume collapse of 10 % at a pressure of 44 to 45 GPa. We investigated changes in the electronic structure of a siderite single crystal for pressures up to 50 GPa using a Boehler-Almax diamond anvil cell with helium as pressure medium by x-ray Raman scattering at the iron $M_{2,3}$-edge and $L_{2,3}$-edge. The course of the spin transition up to 50 GPa is discussed by the observed spectral changes. [1] B. Lavina et al., Geophys. Res. Lett. 36, L23306 (2009)

MM 17.30 Mon 18:00 Poster E

Real space morphological analysis of multilevel domain structures in polycrystalline ferroelectric relaxors — •danka gobeljic[1], vladimir v shvartsman[1], sergei v kalinin[2], stephen jesse[2], and doru c lupascu[1] — [1]Institute for Material Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Essen, Germany — [2]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, USA

The local domain configuration and its dynamics play a vital role in the properties of ferroelectric materials. Therefore, domain architectures have been subject to systematic theoretical and experimental studies. The expected regularity of domain patterns is often distorted in real materials. In particular, this is typical for system with inherent disorder, e.g. for relaxors. Maze-like domain structures have been reported for the latter. To extract quantitative characteristics of such complex domain patterns one needs a special analytical tool. We introduce the quantitative line-of-sight (LoS) domain structure analysis. Based on 2D spatial maps of domain structures obtained by piezoresponse force microscopy (PFM), the LoS provides a quantitative measure of the characteristic domain shape, size, and spatial organization. We demonstrate the validity of this technique for Bi1/2Na1/2TiO3-BaTiO3 based relaxor ceramics. The parameters of the complex domain morphology are discussed in the context of grain orientation and local composition.Beyond comprehensive investigation of the local properties, LoS is applied as a comparative tool in the study of the macroscopic properties of the investigated ceramics.

MM 17.31 Mon 18:00 Poster E

Molecular dynamics simulation of the α-γ phase transition in iron-nickel system — •Emilia Sak-Saracino and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS,Erwin-Schrödinger-Straße, 67663 Kaiserslautern, Germany

Using molecular dynamics simulation, we study the austenite-martensite phase transition in the iron-nickel system. During a heat-

ing/cooling cycle, the phase transition can be observed by monitoring the hysteresis of the system volume with temperature. We find that with increasing nickel concentration, the martensite and austenite temperatures decrease, in agreement with experiment.

MM 17.32 Mon 18:00 Poster E

Theoretical modelling of the electronic structure of MAX phases using WIEN2k and calculation of electric field gradients — Daniel Jürgens[1], Michael Uhrmacher[1], Jose Mestnik-Filho[2], and •Hans Hofsäss[1] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, Sao Paulo, Brazil

Local magnetic fields and electric field gradients at the site of probe atoms in solids can be measured with hyperfine interaction techniques and allows the investigation of the local microstructure around M- and A-sites and possible magnetic properties of MAX-phase compounds. In this work, we us the program WIEN2k to calculate electric field gradients (EFG) for In or Hf probe atoms on either A-or M-sites in different MAX phases. We present comprehensive calculations of EFGs in many 211-MAX phase compounds and compare with our experimental results from perturbed angular correlation measurements. We discuss the dependence of the A-site EFGs as function of the A-Element ranging from Al to Pb and for M-elements ranging from Ti to Hf. We find a characteristic dependence of the EFG strength on the M-element valence electron density. In most of the investigated MAX-phases we can quantitatively predict the EFG for probe atoms on A- or M-sites with good accuracy. This makes perturbed angular correlation an ideal and universal method to study electronic and also possible magnetic properties of MAX phases.

MM 17.33 Mon 18:00 Poster E

Investigations of electric field gradients at A-sites in the 312- and 413-MAX-phases using perturbed angular correlation spectroscopy — Daniel Jürgens[1], Michael Uhrmacher[1], •Hans Hofsäss[1], and Michael W. Barsoum[2] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany — [2]Department of Material Science and Engineering, Drexel University, PA, USA

Local magnetic fields and electric field gradients at the site of probe atoms in solids can be measured with hyperfine interaction techniques and allows the investigation of the local microstructure around M- and A-sites and possible magnetic properties of MAX-phase compounds, which are known for their metallic as well as their ceramic properties. The perturbed angular correlation (PAC) was used to determine the local environment of implanted probe atoms on atomic scale. The compounds Ti_3AlC_2, Ti_3SiC_2, Ti_4AlN_3 and Ta_4AlC_3 were investigated with PAC using implanted 111In probe atoms., which occupy A-sites after annealing the implantation damage. In this study we investigate dependence of the strength of the electric field gradient (EFG) on the stacking sequence of the laminar MAX phases. The comparison of EFGs measured in the different sub-groups of MAX phases show that the EFGs in the 413 phases are slightly smaller compared to the corresponding 211 phase. Increasing the M-X intermediate layer thickness while going from M_2X to M_3X_2 to M_4X_3 phases reduces the EFG strength at the A-Site. This behavior allows a characterization of stacking sequence variations occurring e.g. in thin film MAX phases.

MM 17.34 Mon 18:00 Poster E

Electric field gradients at M- and A-sites in 211 MAX-phases using perturbed angular correlation spectroscopy — Daniel Jürgens[1], Michael Uhmacher[1], Ulrich Vetter[1], Matthias Nagl[1], •Hans Hofsäss[1], Jose Mestnik-Filho[2], and Michael W. Brasoum[3] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, Sao Paulo, Brazil — [3]Department of Material Science and Engineering, Drexel University, PA, USA

Local magnetic fields and electric field gradients at the site of probe atoms in solids can be measured with hyperfine interaction techniques and allows the investigation of the local microstructure around M- and A-sites and possible magnetic properties of MAX-phase compounds, which are known for their metallic as well as their ceramic properties. Since most techniques only allow a macroscopic insight, the perturbed angular correlation (PAC) was used to determine the local environment of implanted probe atoms on atomic scale. Radioactive ^{111}In and ^{181}Hf ions, both decaying by a $\gamma-\gamma$ cascade, were implanted into Zr_2InC and Hf_2InC and the electric field gradients (EFG) at a A-site (in) and M-sites (Hf) were measured after annealing the implantation damage. We report on the different annealing behavior observed for In and Hf probes. We compare the results with density functional theory calculations and give reasons for dissimilar EFGs at A- and M-sites. Further results for other 211 MAX-phases (Ti_2InC, Ti_2AlC, V_2AlC, Cr_2AlC, Nb_2AlC, Ti_2AlN,Cr_2GeC, Ti_2GeC,Nb_2AsC, and Ti_2SiC) are presented.

MM 18: Invited talk Stukowski

Time: Tuesday 9:30–10:00 Location: TC 006

Invited Talk MM 18.1 Tue 9:30 TC 006

Unraveling the Mechanisms of Plasticity in Nanostructured Materials using Advanced Data Analysis and Simulation Methods — •Alexander Stukowski — Institut für Materialwissenschaft, TU Darmstadt

Nanocrystalline, nanotwinned, and nanoporous metals and alloys all exhibit exceptional deformation behavior due to their large density of internal interfaces. Unlike in more coarse-structured materials, a multitude of mechanisms contributes to the plasticity and strength of these novel materials, leading to more complex mechanical behavior.

Large-scale molecular dynamics and new Monte-Carlo simulation methods [1] possess the potential to significantly expand our understanding of the underlying processes that govern the plasticity at the nanoscale. In particular the recent development of sophisticated data analysis algorithms [2] helps us to identify, track, and visualize key microstructural features and defects in complex materials models, leading to new insights into the interplay of competing mechanisms [3] and the internal evolution of materials.

I will highlight several of our recent developments in this active field of research, demonstrate the power of these enabling technologies by looking at different materials systems [4], and discuss challenges yet to be solved in this area of computational materials science.

[1] B. Sadigh et al., Phys. Rev. B 85 (2012), 184203
[2] A. Stukowski, JOM 66, Issue 3 (2014), 399-407
[3] J. Schäfer et al., J. Appl. Phys. 114 (2013), 143501
[4] A. Stukowski, K. Albe, D. Farkas, Phys. Rev. B 82 (2010), 224103

MM 19: Methods in Computational Materials Modelling I: Materials Design

Time: Tuesday 10:15–11:45 Location: H 0106

MM 19.1 Tue 10:15 H 0106

Theory-guided design of high-strength superlattices containing metastable phases: example of nano-scale CrN/AlN — •Martin Friák[1,2], Darius Tytko[1], David Holec[3], Pyuck-Pa Choi[1], Philip Eisenlohr[1], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., Brno, Czech Republic — [3]Montanuniversität Leoben, Leoben, Austria

A theory-guided materials design of nano-scaled superlattices containing metastable phases is critically important for future development of advanced lamellar composites. Our study combining theoretical and experimental methods exemplifies this approach in the case of elastic properties of AlN/CrN superlattices with a bilayer period of 4 nm in which CrN stabilizes AlN in a metastable B1 cubic phase. As B1-AlN crystals do not exist as bulk material at ambient pressure, experimental data for this phase are not available. Therefore, quantum-mechanical calculations have been applied to simulate an AlN/CrN superlattice. The ab initio predicted Young's modulus (428 GPa) in a direction perpendicular to (001) oriented interfaces is in excellent agreement with measured nano-indentation value (408 +/- 24 GPa). Aiming at a future rapid high-throughput design of superlattices, we have also tested predictions obtained within linear-elasticity continuum modeling that employs elastic properties of B1-CrN and B1-AlN phases as input. Using single-crystal elastic constants from ab initio calculations for both phases, we discuss the accuracy of this approach, too.

MM 19.2 Tue 10:30 H 0106

Big Data of Materials Science - Critical Role of the Descriptor — •Luca M. Ghiringhelli[1], Jan Vybiral[2], Sergey V. Levchenko[1], Claudia Draxl[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Charles University, Prague, CZ — [3]Humboldt-Universität zu Berlin, Berlin, DE

Statistical learning of materials properties or functions so far starts with a largely silent, non-challenged step: the introduction of a multidimensional descriptor. However, when the scientific relationship of the descriptor to the actuating mechanisms is unclear, causality of the trained (learned) descriptor-property relation is uncertain. Thus, scientific advancement, trustful prediction of new promising materials and identification of anomalies is doubtful. We discuss and analyze this issue and define requirements for a descriptor that is suited for statistical learning of materials properties and functions. We show how a meaningful descriptor can be found systematically, by means of compressed sensing techniques. These concepts are demonstrated for examples in materials science: prediction of the relative stability of zincblende/wurtzite vs rocksalt octet binary semiconductors, and prediction of their band gaps, by using simple atomic input for building the descriptor.

MM 19.3 Tue 10:45 H 0106

Accurate Thermal Conductivities from First Principles — •Christian Carbogno and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

In spite of significant research efforts, a first-principles determination of the thermal conductivity at high temperatures has remained elusive. Boltzmann transport techniques that account for anharmonic effects only perturbatively become inaccurate or inapplicable under such conditions; non-equilibrium molecular dynamics (MD) methods suffer from enormous finite-size artifacts in the computationally feasible supercells. Using Green-Kubo theory [1], we overcome this limitation by performing equilibrium *ab initio* MD simulations, from which the thermal conductivity is assessed from the auto-correlation function of the heat flux (including anharmonic effects to all orders). Foremost, we introduce and discuss a first-principles definition of the heat flux using the virial theorem. We validate our approach and in particular the techniques developed to overcome finite time and size effects, e.g., by inspecting silicon, the thermal conductivity of which is particularly challenging to converge [2]. Furthermore, we investigate the thermal conductivity of ZrO_2, which is known for its high degree of anharmonicity. Our calculations shed light on the heat resistance mechanism active in this material, which eventually allows us to discuss how the thermal conductivity can be controlled by doping [3].

[1] R. Kubo, *et al.*, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).
[2] Y. He *et al.*, *Phys. Chem. Chem. Phys.* **14**, 16209 (2012).
[3] C. Carbogno, *et al.*, *Phys. Rev. B* **90**, 144109 (2014).

MM 19.4 Tue 11:00 H 0106

Structure map for crystal-structure prediction of sp-d valent compounds — Arthur Bialon, •Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges of materials design. We present a three-dimensional structure map based on experimental data for compounds that contain sp-block elements and transition metals. The map predicts the correct crystal structure with a probability of 86% and has a confidence of 98% that the correct crystal structure is among a candidate list of three crystal structures. The three order parameters of the structure map are physically intuitive functions of the number of valence electrons, atomic volume and electro-negativity of the constituent elements. We test the structure map against standard density functional theory calculations for 1:1 sp-d-valent compounds and demonstrate that our three-parameter model has a comparable predictive ability. We show that the structure map can be applied to off-stoichiometric compounds and extended to ternary crystal-structure prototypes.

MM 19.5 Tue 11:15 H 0106

Property-based *cascade* genetic algorithms for tailored searches of metal-oxide nano-structures — •Saswata Bhattacharya[1], Luca M. Ghiringhelli[1], and Noa Marom[2] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Tulane University, New Orleans, LA, USA

There is considerable interest in the computational determination of structures of atomic clusters that are detected in spectroscopy experiments. It has been suggested that in photo-emission experiments performed on anions, isomers of small $(TiO_2)_n$ clusters with high electron affinity (EA) are selectively observed rather than those with the lowest energy [1]. For the theoretical modeling of these situations, searching for the energy global minimum of the potential energy surface (PES) is inefficient. By using such an approach, in fact, it is unlikely to find meta-stable isomers that have high EA or low ionization potential (IP), but energy significantly above the ground state. We present an extension to our recently developed *ab initio* cascade genetic algorithm [2], here tailored to conduct property-based (e.g., high EA, low IP) searches over the PES. The term *cascade* refers to a multi-stepped algorithm where successive steps employ a higher level of theory, and each step of the next level takes information obtained at the immediate lower level. The new algorithms are benchmarked and validated for $(TiO_2)_n$ clusters ($n = 3 - 10, 15, 20$). − [1] N. Marom *et al.* Phys. Rev. Lett. **108**, 106801 (2012) [2] S. Bhattacharya *et al.*, New J. Phys., in press (2014).

15 min. break

MM 20: Liquid and Amorphous Metals III: Deformation of Metallic Glasses

Time: Tuesday 10:15–11:30 Location: H 0107

MM 20.1 Tue 10:15 H 0107

Potential energy landscape of deformed Cu-Zr based metallic glasses — •Tobias Brink and Karsten Albe — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Metallic glasses are usually described in terms of a potential energy landscape which consists of large megabasins that contain small local minima with low barriers between them. In this work, we explore the potential energy landscape of Cu-Zr glasses of varying composition using an adaptive kinetic Monte Carlo method with high temperature molecular dynamics saddle-point search. We examine the evolution of the potential energy landscape under applied strain and identify transient structural excitations as well as stress-activated plastic events (shear transformation zones). We make a distinction between these events and classify them in terms of their barriers and structural changes. Using this data, we gain quantitative insights into the microscopic processes of plastic deformation in metallic glasses, which ultimately lead to the percolation of a shear band.

MM 20.2 Tue 10:30 H 0107

Avalanches dynamics and microstructure evolution of the glassy Cu50Zr50 system by means of Molecular Dynamic Simulations. — •Alexandra Lagogianni and Konrad Samwer — 1. Physikalisches Institut, Universität Göttingen, Germany

Several experimental studies revealed the presence of avalanches/stress drops in the plastic regime of BMGs, [1-3] upon mechanical deformation, and their direct correlation with the formation and arrest of single shear bands. Aiming to gain a deeper insight of this phenomenon on a smaller length scale we employed molecular dynamic 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 were statistically analysed. In agreement with the experimental findings 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 theoritical confirmation of the experimental findings and a deeper and qualitative understanding of the origin of avalanches in a metallic glass.

MM 20.3 Tue 10:45 H 0107

Investigation of kinetics and strain fields in shear bands of a Pd40Ni40P20 bulk metallic glass — •Isabelle Binkowski, Sergiy Divinski, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

Bulk metallic glasses feature beneficial properties which are promising for applications, because of which they have reached increasing attention. Metallic glasses exhibit mechanical properties such as high strength and hardness, however, this advantage is impeded by the fact that their plasticity appears to be extremely limited. At temperatures well below the glass transition, the plastic deformation is localized in thin regions, called shear bands, with widths from 5 nm to 50 nm, whose continued activation leads to a catastrophic failure. In the area of research on shear bands, several important questions are still open, as e.g. concerning the initiation, propagation, kinetics of shear banding as well as concerning the intrinsic properties of these thin plate-like regions. In the present study, the mechanism of shear banding in a Pd40Ni40P20 bulk metallic glass was investigated in detail. The investigation focuses on the kinetic and structural properties of the shear bands in this highly stable bulk metallic glass by the use of various experimental techniques.

MM 20.4 Tue 11:00 H 0107

Crossover from random three-dimensional avalanches to correlated nano shear bands in metallic glasses — •Carlos Herrero-Gómez, Jon-Olaf Krisponeit, Sebastian Pitikaris, Karina E.Avila, Stefan Küchemann, Antje Krüger, and Konrad Samwer — University of Goettingen,Goettingen, Germany

Bulk metallic glasses respond with elastic and/or plastic deformation to applied mechanical stresses. Such deformation do not have a smooth dependence with the applied stress but take place via jerky jumps, which are often referred as Crackling Noise [1] . We report a statistical analysis of the crackling noise in metallic glasses for creep measurements. Such analysis shows the existence of a crossover which seems to indicate a change in the process of deformation [2]. Although the microscopic theory of deformation remains an open task, this crossover seems to indicate a transition in the plastic deformation behavior from the three-dimensional random activity of Shear Transformation Zones to a two-dimensional nano-shear band sliding. Financial support by the EU Marie Curie Grant 60780 within the VitriMetTech Initial Training Network is thankfully acknowledged.

[1] Dahmen, Karin Ben-Zion, Yehuda Uhl, Jonathan. Micromechanical Model for Deformation in Solids with Universal Predictions for Stress-Strain Curves and Slip Avalanches. Phs Rev Let.102,17, 175501 (2009)

[2] Krisponeit, J.O et al. Crossover from random three-dimensional avalanches to correlated nano shear bands in metallic glasses. Nat. Commun. 5:3616 (2014)

MM 20.5 Tue 11:15 H 0107

Evolution of crystallite size, lattice parameter and internal strain in Al precipitates during high energy ball milling of partly amorphous Al87Ni8La5 alloy — •Matthias Dittrich[1,2] and Gerhard Schumacher[1] — [1]Helmholtz-Zentrum Berlin, Mikrostruktur und Eigenspannungsanalyse — [2]jetzt: Bundesanstalt für Materialforschung und -Prüfung Berlin

The effects of plastic deformation by ball milling on the structure of a partly amorphous Al87Ni8La5 alloy were investigated by X-ray diffractometry. Lattice parameter, crystallite size and lattice strain of the fcc-Al precipitates were determined by Rietveld refinement, double-Voigt approach and Williamson-Hall plots. The changes in lattice parameter of fcc-Al nano-precipitates during ball milling are ascribed to the uptake of Ni. The crystallite size decreases as a function of the milling time from about 100 nm in the as- atomized state to about 14 nm after 1440 min of ball milling time. A model based on shear deformation of precipitates in the amorphous phase is used to describe quantitatively the decrease in crystallite size and change in lattice parameter.

MM 21: Hydrogen in metals IV: Special topics

Time: Tuesday 10:15–11:45 Location: TC 006

Topical Talk MM 21.1 Tue 10:15 TC 006

Hydrogenography and Metalhydride Switchable Mirrors — •Ronald Griessen — VU university, Amsterdam, The Netherlands

The discovery [1] of dramatic optical changes in metallic films loaded with hydrogen opened the way to Hydrogenography [2]. The great advantage of this new high-throughput technique is to measure optically and simultaneously on thousands of (nano)structured samples, pressure-composition isotherms, enthalpies and entropies of hydride formation. Hydrogenography provides also unique possibilities to measure reaction kinetics and catalytic activities, long-range diffusion [3], the intrinsic hydrogen permeability of alloys [4], and to optimize switchable metal-hydrides for smart windows, optic hydrogen sensors [5] and nanoantennas for active plasmonics [6].

[1] J.N. Huiberts, et al., Nature 380 (1996) 231-234; [2] R. Gremaud, et al., Advanced Materials 19 (2007)2813; [3] A. Remhof, et al., Physical Review Letters 90 (2003) 145502; [4] S. de Man et al., J. Membrane Science 444(2013)70; [5] P. Ngene et al., Adv. Funct. Mater. 2014, 24, 2374; [6] N. Strohfeldt et al., Nano Lett. 14 (2014) 1140.

MM 21.2 Tue 10:45 TC 006

A novel method for detecting hydrogen in metals at high local resolution and with ultra-high sensitivity — •Michael Rohwerder — Max-Planck-Institut für Eisenforschung GmbH

Already very low hydrogen concentrations can cause hydrogen embrittlement of high strength materials. In this presentation a novel method will be presented that allows the spatially resolved, ultra-sensitive measurements of hydrogen in steels and other alloys as well as its uptake into and permeation through them [1-4]. Several examples demonstrating the capabilities of this novel, Kelvin probe based technique will be presented. Finally, an example will be given demonstrating the role of localized hydrogen enrichments for hydrogen embrittlement of TWIP steels.

References:

[1] C. Senöz, S. Evers, M. Stratmann and M. Rohwerder, Electrochem. Commun. 13 (2012)1542

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[3] S. Evers, S. Ceylan, M. Rohwerder, Science and Technology of Advanced Materials 14 (2013) 014201

[4]S. Evers, C. Senöz, M. Electrochimica Acta 110 (2013) 534

MM 21.3 Tue 11:00 TC 006

Thermal desorption spectra from 3D materials — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Temperature programmed desorption (TPD) is frequently used in surface science to characterise adsorption sites and reactions on surfaces. It can also be applied to bulk materials to study the trapping of solute atoms at point and extended defects, such as vacancies, grain boundaries or dislocations. Using a kinetic Monte Carlo (kMC) approach to simulate TPD spectra for surfaces has provided valuable information for the interpretation of the different contributions to the spectra.

Here we simulate TPD spectra for bulk systems. The kMC Model consists of a 3D lattice with a surface and we include the effect of bulk diffusion on the TPD spectra. The effect of various defects on diffusion and the resulting desorption spectra are analysed.

MM 21.4 Tue 11:15 TC 006

Chemical Trends Of Interstitial Solubility In Transition Metals: DFT Driven High-Throughput Databases — •Ugur Aydin, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

We present insights for chemical trends of the solubility of interstitial elements H, He, B, C, N, O, F, Ne in 3d, 4d, 5d transition metals obtained with High-Throughput DFT calculations. The parallel generation of the bulk-interstitial systems and their systematic investigation with an in-house developed workbench, called *pyCMW*, allowed us to classify the elastic and chemical mechanisms governing the solution enthalpy of the interstitials mentioned above. The introduction of a correlation coefficient $r_{xy} \in [0, 1]$ between the bulk modulus B_0 and the solution enthalpy ΔH gives a qualitative insight for both mechanisms. While for non-reactant interstitial elements, the noble gases He and Ne, $r_{xy} = 0.97$ indicates a very high elastic but a very low chemical impact on ΔH, interstitial hydrogen shows with $r_{xy} = 0.03$ (very high chemical but very low elastic contribution) an inverse behavior. In a similar way all interstitial elements can be ordered according to the chemical and elastic impact on ΔH.

15 min. break

MM 22: Functional Materials IV: Thermoelectric and Multiferroic Materials

Time: Tuesday 10:15–11:45 Location: TC 010

MM 22.1 Tue 10:15 TC 010

Thermoelectric properties of the layered rhodates K_xRhO_2 and Na_xRhO_2 — •Udo Schwingenschlögl, Yasir Saeed, and Nirpendra Singh — KAUST, Thuwal 23955-6900, Saudi Arabia

The thermoelectric properties of the layered oxides K_xRhO_2 ($x = 1/2$ and $7/8$) are investigated by means of the electronic structure, as determined by ab inito calculations and Boltzmann transport theory. In general, the electronic structure of K_xRhO_2 is similar to Na_xCoO_2, but with strongly enhanced transport. $K_{7/8}RhO_2$ exceeds the ultra-high power factor of $Na_{0.88}CoO_2$ reported previously by more than 50%. The roles of the cation concentration and the lattice parameters in the transport properties in this class of compounds are explained. In addition, we study the 3R phases of Na_xRhO_2 for different Na vacancy configurations and concentrations. As compared to the analogous 2H phases, the modified stacking of the atomic layers in the 3R phases reduces the interlayer coupling. As a consequence, the 3R phases are found to be superior in the technologically relevant temperature range. The Rh $d_{3z^2-r^2}$ orbitals still govern the valence band maxima and therefore determine the transport properties. A high figure of merit of 0.35 is achieved in hydrated $Na_{0.83}RhO_2$ at 580 K by water intercalation, which is 34% higher than in the non-hydrated phase. References: Adv. Funct. Mater. 22, 2792 (2012); Sci. Rep. 4, 4390 (2014).

MM 22.2 Tue 10:30 TC 010

Thermoelectric properties of individual Ag nanowires under the terms of quasiballistic transport — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[2], Johannes Ruhhammer[2], Peter Woias[2], and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt Universität zu Berlin, D-12489 Berlin, Newtonstr. 15 — [2]Laboratory of Design of Microsystems, University of Freiburg, IMTEK, D-79110 Freiburg

The thermoelectric properties of Ag nanowires (NW) are discussed as a function of temperature T. Especially the electrical conductivity and the thermal conductivity showed reduced values with respect to the bulk. The latter are both notably dominated by surface scattering due to an increased surface-to-volume ratio. By lowering T, the electron mean free path strongly exceeds the NW's diameter of 150nm so that the transition from diffusive transport to quasi ballistic transport is observed. Whereas the conductivities are influenced by the NW's diameter the Lorenz number L(T) turns out to be independent of surface scattering. Instead of that, the characteristic of L(T) is determined by the material's purity. Moreover, the temperature dependence of the electrical conductivity and L(T) can be described by the bulk Debye temperature of silver.

MM 22.3 Tue 10:45 TC 010

Vibrational dynamics of filled skutterudites: Role of the fillers — •Susmita Basak, Christian Carbogno, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Skutterudites are regarded as potential candidates for next-generation thermoelectric materials for electrical power generation using either

solar energy or waste heat [1,2]. They form open cage-like covalent structures with large interstitial voids that can accommodate filler atoms. In principle, the thermoelectric efficiency of skutterudites can be tailored and improved in presence of these foreign atoms because different filler species affect the vibrational and electronic transport coefficients differently. In order to rationalize this phenomenon, various (in part mutually exclusive) mechanisms (rattling of filler atoms [3], hybridization between guest and host atoms [4] etc.) have been evoked in literature. To shed light on the underlying interactions, we use density functional theory to systematically study the electronic structure and the lattice dynamics of skutterudites (CoSb3, CoAs3 etc,) with various fillers (Ba, Ga, In, Sn etc.). We incorporate the full anharmonicity of the inter-atomic interactions via *ab initio* molecular dynamics techniques. Our calculations reveal a unified mechanism that determines the dynamics and hence provide insights/guidelines to engineer the vibrational band structure in this material class.

[1] B. C. Sales *et al.*, Science **272**, 1325 (1996). [2] G. S. Nolas *et al.*, Phys. Rev. B, **58**, 164 (1998). [3] G. A. Slack *et al.*, J. Appl. Phys. **76**, 1665 (1994). [4] J. L. Feldman *et al.*, Phys. Rev. B **61**, R9209 (2000).

MM 22.4 Tue 11:00 TC 010

Microscopic model of paralectric/ferroelectric perovskites — •Giovanni Pizzi[1], Andrea Cepellotti[1], Boris Kozinsky[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), EPFL (CH) — [2]Robert Bosch LCC Research and Technology Center, Cambridge (USA)

Even if ferroelectric materials like $BaTiO_3$ have been used for decades in a broad range of technological applications, there is still significant debate in the literature concerning their microscopic behavior. In particular, many perovskite systems display a high-temperature cubic phase with zero net polarization, whose microscopic nature is though still unclear. Indeed, some of these perovskite systems display a complex energy landscape with multiple local minima. Using our high-throughput platform AiiDA (www.aiida.net) to manage all calculations, we perform a study on a set of representative ABO_3 perovskites. We use spacegroup techniques to systematically analyze all possible local displacement patterns that are compatible with a net paraelectric phase, together with DFT calculations to assess the energetics and the stability of these patterns. Using this technique, we are able to describe the different classes of microscopic models underlying the perovskite systems.

MM 22.5 Tue 11:15 TC 010

Design of a Mott Multiferroic from a Non-Magnetic Polar Metal — •Gianluca Giovannetti[1], Danilo Puggioni[2], James Rondinelli[2], and Massimo Capone[1] — [1]CNR-IOM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136, Trieste, Italy — [2]Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

Metals are expected to not exhibit ferroelectricity because static internal electric fields are screened by conduction electrons. A class of materials known as "ferroelectric metals" was discussed theoretically by Anderson and Blount in 1965 [1]. Recently $LiOsO_3$ has been found to be a "ferroelectric metal" in the sense that it is a metal but it develops a broken-symmetry ionic structure [2]. Using a combined approach based on Density Functional Theory and Dynamical Mean Field Theory we address the driving force behind the ferroelectric instability in metallic $LiOsO_3$ and we show that the metallic state of $LiOsO_3$ is controlled by the amount of the electronic correlations of the t_{2g} states of Os. We unreveal how the effect of correlations of this compound can be tuned to engineer a Mott Multiferroic state in Li_2NbOsO_6 1/1 superlattice. We find Li_2NbOsO_6 1/1 superlattice to be a type-II multiferroic material with large ferrolectric polarization and Néel temperature close to room temperature.

[1] Anderson and Blount, Phys. Rev. Lett. 14, 217 (1965). [2] Y. Shi et Al. Nat. Mat. 12, 1024 (2013).

15 min. break

MM 23: Methods in Computational Materials Modelling: Battery Mateirals

Time: Tuesday 11:45–12:45 Location: H 0106

MM 23.1 Tue 11:45 H 0106

Electronic structure of oxygen-deficient $Li_4Ti_5O_{12-\delta}$ — Saskia Stegmaier, •Christoph Scheurer, and Karsten Reuter — Technische Universität München, Germany

The lithium titanate $Li_4Ti_5O_{12}$ (LTO) is a promising alternative anode material for rechargeable lithium-ion batteries which offers advantageous materials properties in terms of safety and stability. The low electronic conductivity of pristine $Li_4Ti_5O_{12}$, however, is a drawback. LTO samples with an increased electronic conductivity have been prepared, for example, via routes including thermal treatment in reducing atmosphere. Under these conditions, oxygen vacancies are formed and Ti^{4+} ions are reduced. Experimental XPS and EPR data indicate the presence of discrete Ti^{3+} and Ti^{4+} ions rather than a full delocalization of the extra electrons.[1,2] Such oxygen-deficient materials with mixed-valent metal cations pose a challenge to computational materials modeling with density-functional theory (DFT) methods since calculations with standard LDA or GGA functionals only lead to a delocalized picture of the charge distribution. DFT+U calculations can be employed to capture spatial localization of excess electrons on transition metal sites but the choice of the Hubbard U parameter introduces some ambiguity. We thus performed DFT calculations with hybrid functionals in order to gain a more reliable first principles based insight into the defect chemistry and electronic structure of oxygen-deficient $Li_4Ti_5O_{12-\delta}$.

[1] J. Wolfenstine, J. L. Allen, *J. Power Sources* **2008**, *180*, 582.
[2] H. Song et al., *Sci. Rep.* **2014**, *4*, 4350.

MM 23.2 Tue 12:00 H 0106

Assessing PAW pseudopotentials for solid-state NMR calculations — •Ary Ferreira, Karsten Reuter, and Christoph Scheurer — Technische Universität München

The Gauge-Including (GI) Projector Augmented Wave (PAW) method [1] allows for an efficient simulation of solid-state Nuclear Magnetic Resonance (NMR) spectra within a density-functional theory framework. It derives its efficiency by calculating the all-electron magnetic response with frozen-core PAW pseudopotentials. The accuracy of GIPAW calculated nuclear magnetic shieldings and electric field gradients is correspondingly critically determined by the quality of these PAW potentials. Here we assess this quality for a range of metal oxides of differening covalency in the metal-O bond by comparing to reference full-potential calculations performed within the LAPW/APW+lo method. We compute correlations between NMR parameters and isotropic changes in each MO_n coordination environment [2] to propose the use a single number to systematically express the difference between results obtained with the two methods. [1] C.J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001). [2] K. Lejaeghere *et al.*, Crit. Rev. Solid State Mater. Sci. **39**, 1 (2014).

MM 23.3 Tue 12:15 H 0106

DFT-based reference parameters for solid-state NMR on Li-ion batteries — •Simone Köcher[1,2], Rüdiger Eichel[1], Karsten Reuter[2], and Christoph Scheurer[2] — [1]IEK-9, Forschungszentrum Jülich — [2]Technische Universität München

In-operando Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool to gain a detailed understanding of the fundamental dynamical processes inside an operating battery cell [1]. Notwithstanding, the experimental spectra are complex and their unambiguous interpretation has to rely on independent first-principles based simulations. For studies of the ionic charge carrier mobility in Li-ion batteries by ^{6,7}Li solid-state NMR, corresponding simulations require an accurate reference scale of different lithium compounds. We establish these NMR parameters through density-functional theory (DFT) calculations for ideal periodic lithium salts as well as for some organolithium compounds [2]. We specifically explore the influence of geometry, symmetry and computational method on the calculated chemical shieldings and address the challenges involved in simulating disordered materials.

[1] B. Key *et al.*, J. Am. Chem. Soc. **131**, 9239 (2009); [2] C. Bonhomme *et al.*, Chem. Rev. **112**, 5733 (2012).

MM 23.4 Tue 12:30 H 0106

Phase field modeling of Li-insertion kinetics in single $LiFePO_4$- nano-particles for rechargeable Li-ion battery application — •Michael Fleck, Holger Federmann, Philipp Amendt, and Heike Emmerich — Materials and Processsimulation, University of Bayreuth

$LiFePO_4$ 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. 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.

MM 24: Transport II: Thermal and Electrical Conductivity

Time: Tuesday 11:45–12:45 Location: H 0107

MM 24.1 Tue 11:45 H 0107

Thermal conductivity of half-Heusler thermoelectric materials from first principles — •Lars Bergqvist — Dept. of Materials and Nano Physics, KTH Royal Institute of Technology, Electrum 229, SE-164 40 Kista, Sweden — Swedish e-Science Research Centre (SeRC), KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Thermal conductivity and finite temperature phonon properties of half-Heusler thermoelectric materials are presented using large-scale ab-initio molecular dynamics simulations for calculation of interatomic force constants (IFC), including temperature and anharmonic effects, together with the full solution of the Boltzmann transport equation for phonons, as implemented in the newly developed Temperature Dependent anharmonic Effective Potential (TDEP) methodology.

Calculated lattice thermal conductivity, important for thermoelectric performance, show good agreement with experimental data. In particular, it is found that n-type ZrNiSn has lower conductivity than p-doped ZrCoSb, which can be analyzed in terms of the phonon lifetimes and broadening of the spectra from the dynamic structure factor at finite temperatures. Moreover, doping with Hf in ZrNiSn further reduces the thermal conductivity.

MM 24.2 Tue 12:00 H 0107

Microscopic theory and ab initio simulation of atomic heat transport — •Aris Marcolongo[1], Stefano Baroni[2], and Paolo Umari[3] — [1]Ecole Polytechnique Federale de Lausanne, Switzerland — [2]SISSA – International School for Advanced Studies, Trieste, Italy — [3]Department of Physics and Astronomy, Padua University, Italy

Green Kubo formulas, combined with classical molecular dynamics, are often used to compute thermal conductivity coefficients of liquid systems. Nevertheless, application to ab-initio molecular dynamics is often believed to be problematic because a suitable quantum-mechanical definition of the heat current is not readily available, due to the ill-definedness of the microscopic energy density to which it is related by the continuity equation. We argue that a similar difficulty actually exists in classical mechanics as well and show that it is nevertheless possible to obtain a physically well defined transport coefficient, independent of the ill defined microscopic energy density. We then derive an expliticit expression for the adiabatic energy current within density-functional theory, well defined under periodic boundary conditions. The resulting methodology is demonstrated by comparing ab initio and classical molecular simulations of a model liquid-Argon system, for which accurate inter-atomic potentials are derived by the force-matching method.

MM 24.3 Tue 12:15 H 0107

Topological insulators defined by local and non-local resistivity — •C. Shekhar[1], S. Ouardi[1], C. E. ViolBarbosa[1], B. Yan[1,2], W. Schnelle[1], G. H. Fecher[1], and C. Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for Physics of the Complex Systems, 01187 Dresden, Germany

Topological insulators are known for their metallic surface states, a result of strong spin-orbit coupling, that exhibit unique surface transport phenomenon. However, these surface transport phenomena are buried in the presence of metallic bulk conduction. We synthesized very high quality Bi_2 Te_2 Se single crystals by using a modified Bridgman method that possess high bulk resistivity of >20 Omega cm below 20K, whereas the bulk is mostly inactive and surface transport dominates. The temperature dependence of resistivity follows an activation law like a gap semiconductor in temperature range 20-300K. To define the topological property i.e. extract the surface transport from that of the bulk, we designed a special measurement geometry to measure the resistance in local and non-local regions. We find that single-crystal Bi_2 Te_2 Se exhibits a crossover from bulk to surface conduction at 20K. Simultaneously, the material also shows strong evidence of surface transport in magneto-conductance. This novel simple geometry facilitates finding evidence of surface transport in topological insulators, which are promising materials for future spintronic applications.

MM 24.4 Tue 12:30 H 0107

crystal growth, resistivity and hall effect of the delafossite metal PtCoO2 — pallavi kushwaha[1], philip moll[2], •nabhanila nandi[1], and andrew mackenzie[1,3] — [1]1 Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straβe 40, 01217 Dresden, Germany — [2]Laboratory for Solid State Physics, ETH Zurich, Switzerland — [3]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We report single crystal growth of the delafossite oxide PtCoO2, and basic transport measurements on single crystals etched to well-defined geometries using focused ion beam techniques. The room temperature resistivity is 2.1 $\mu\Omega$cm, and the Hall coefficient is consistent with the existence of one free electron per Pt. Although the residual resistivity ratio is greater than fifty, a slight upturn of resistivity is seen below 15 K. The angle dependence of the in-plane magnetoresistance is also reported.

MM 25: Hydrogen in Metals V: H in Steels

Time: Tuesday 11:45–13:15 Location: TC 006

Topical Talk MM 25.1 Tue 11:45 TC 006

An Industrial Perspective on Materials Design for Reduced Sensitivity to Hydrogen-Embrittlement — •Richard G. Thiessen and Oliver Rott — ThyssenKrupp Steel Europe AG, Duisburg, Germany

In order to improve efficiency, performance and safety in the automobile and transportation sector, manufacturers require materials with higher strengths while maintaining or improving their ductility. These demands are being met with extremely complex steels which exploit thermodynamically meta-stable phases to expand the property combinations. The resulting microstructures are challenging to characterize with even the most advanced techniques, let alone the investigation towards their interaction with hydrogen. Nevertheless, advances have been made in recent years in linking details in the microstructure to the behavior of hydrogen in these microstructures. The presented research aims to show some typical demands of modern advanced high strength steels, illustrate typical setups for the testing and measurement of hydrogen, and to correlate trends in the testing results with features in the microstructure. Furthermore, some suggestions and considerations will be given for the development of new steels with a reduced sensitivity to hydrogen-embrittlement.

MM 25.2 Tue 12:15 TC 006

Influence of hydrogen on the fatigue strength of ferritic stainless steel — •Andrej Turk[1], Georg Schauer[2], and Ferdinand Haider[3] — [1]Technische Universität München — [2]Robert Bosch GmbH — [3]Universität Augsburg

In this work the fatigue behaviour of 1.4005IA stainless ferritic steel is investigated. Stress S-N and strain S-N curves are obtained with respect to two parameters: load ratio R and surface residual stresses. Air-tested specimens are compared to specimens electrochemically precharged with hydrogen and tested in a gaseous hydrogen atmosphere of 10 bar. The fracture surfaces of broken specimens are analysed to determine the nature of the failure, its point of origin and how the surface is related to the experimental parameters. While such observations have been reported for a variety of high-strength steels and austenitic steels, little information on ferritic stainless steels is available to date. Additionally, TDS measurements of precharged specimens are carried out to investigate hydrogen distribution in the microstructure and hydrogen saturation kinetics. A review of hydrogen embrittlement mechanisms under static loading is given and used to evaluate the experimental results. The applicability of these mechanisms to cyclic loading conditions is discussed as well as their likelihood in this particular case.

MM 25.3 Tue 12:30 TC 006

Eigenschaftsdegradation durch H in schweißgeeigneten höherfesten Feinkornbaustählen unterschiedlicher Herstellungsverfahren — •Enrico Steppan, Arne Kromm und Thomas Kannengiesser — Bundesanstalt für Materialforschung und -prüfung

Der Einsatz schweißge. höherfester FKB ist aus wirtschaftlichen Gründen & dem Streben nach konstruktivem Leichtbau in vielen Industriezweigen unabdingbar. Das Potential einer Sensibilität gegenüber H-bedingter Eigenschaftsdeg. ist jedoch signifikant erhöht. Die mech.-technolog. Gütewerte moderner niedriglegierter höherfester FKB werden maßgeblich durch Ihre chem. Zus. und dem Herstellungsprozess beeinflusst. Hierdurch leiten sich mikrostrukturelle Unterschiede (Korngröße, Ausscheidungen, Versetzungen) ab. Aufgrund dessen wurden 2 höherf. FKB gleicher Festigkeitsklasse, jedoch unterschiedlicher Herstellung (vergütet Q/thermomechanisch MC), untersucht. Neben den makroskopisch beobachtbaren Merkmalen (Streckgrenzenerhöhung, Abnahme wahre Bruchdehnung und Bruchfläche) wurde das lokale Verhalten unter H in den Stählen mit Synchrotronstrahlung am HZB untersucht. Anhand H-beladener Zugproben wurde die Wechselwirkung des H mit dem Gitter untersucht. Hierzu wurden entsprechende Messungen während des Zugversuches im elast., elast./plast. und plast. Bereich vorgenommen. Grundlegende Unterschiede zwischen den verwendeten Stahlgüten bezüglich der H-degradation ließen sich somit anhand makroskopischer als auch mikroskopischer Merkmale erstmals belegen. Die erlaubt schließlich Rückschlüsse auf die grundlegenden Mechanismen der Eigenschaftsdeg. durch H.

MM 25.4 Tue 12:45 TC 006

The impact of carbides on the hydrogen trapping and embrittlement of Fe-C-X quenched and tempered alloys — •Tom Depover[1], Elien Wallaert[1], Zinedine Zermout[2], and Kim Verbeken[1] — [1]Department of Materials Science and Engineering, Ghent University, Belgium — [2]ArcelorMittal Global R&D Ghent, Zelzate, Belgium

The present work evaluates hydrogen trapping and embrittlement of different laboratory cast Fe-C-X alloys with various carbide forming elements (=X). Tempering generated X-based precipitates. The materials were examined under two conditions, as quenched and quenched and tempered. The hydrogen trapping capacity of the precipitates was investigated by thermal desorption spectroscopy, while melt extraction allowed to determine the hydrogen content after cathodic charging. In-situ hydrogen pre-charged tensile tests were performed to evaluate the hydrogen embrittlement susceptibility. The different carbides exhibited a variable effect on the hydrogen embrittlement behavior. For example, the Fe-C-Ti material embrittled the most and tempering even increased its susceptibility, whereas the opposite tendency was observed for the Fe-C-Cr grade. On the contrary, the resistance against embrittlement was good for all Fe-C-Mo alloys. Other carbide forming elements such as V, Nb and W were evaluated as well. All observations were correlated with thermal desorption spectroscopy and melt extraction results. It was also demonstrated that, by modifying the tempering treatment, the Ea of the traps could be increased and hence the HE-resistance of the material was improved.

MM 25.5 Tue 13:00 TC 006

Die Bestimmung von Wasserstoffverteilungen in Eisen und Stahl mittels Neutronenradiographie und -tomographie — •Axel Griesche, Thomas Schaupp und Thomas Kannengiesser — BAM Federal Institute for Materials Research and Testing, Berlin, Germany

Wir zeigen die Ergebnisse von neutronentomographischen Messungen von Wasserstoffverteilungen in zentimeterdicken Stahl- und Eisenproben. Es gelang die Messung von Wasserstoffverteilungen an Rissflanken in wasserstoffversprödeten Eisenproben [1] mit einer Ortsauflösung in den rekonstruierten 3D-Modellen von ca. 25E-6 m. Dabei konnte auch erstmals gasförmiger Wasserstoff in den Hohlräumen der Risse nachgewiesen und dessen Druck bestimmt werden. Die verwendete Messmethode wird der häufig verwendeten Trägergas-Heißextraktion gegenüber gestellt [2]. Die Neutronenmessungen wurden an den Forschungsreaktoren BER II des HZB in Berlin und FRM II der Neutronenquelle Heinz Maier-Leibnitz in Garching durchgeführt.

[1] Griesche A, Dabah E, Kardjilov N, Hilger A, Manke I, Kannengiesser T, Three-dimensional imaging of hydrogen blister in iron with neutron tomography, Acta Mater 78 (2014) 14

[2] Griesche A, Solórzano E, Beyer K, Kannengiesser T, The advantage of using in-situ methods for studying hydrogen mass transport: Neutron radiography vs. carrier gas hot extraction, Int J Hydrogen Energy 38 (2013) 14725

MM 26: Functional Materials V: Functional Materials

Time: Tuesday 11:45–13:00 Location: TC 010

MM 26.1 Tue 11:45 TC 010

Neutron Imaging of Metal Hydride based Hydrogen Storage Tanks — •Stefan Börries[1], Philipp Klaus Pranzas[1], Oliver Metz[1], Martin Dornheim[1], Thomas Bücherl[2], Thomas Klassen[1], and Andreas Schreyer[1] — [1]Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research, Max-Planck-Straße 1 D-21502 Geesthacht, Germany — [2]ZTWB Radiochemie München (RCM), Technische Universität München (TUM), Walther-Meissner-Str. 3, 85748 Garching, Germany

Hydrogen is a promising energy carrier for the future, especially for mobile applications. It can be stored safely and reversibly at high volumetric densities in hydrogen storage tanks filled with light metal hydrides. Due to the high sensitivity of neutrons towards hydrogen, Neutron Radiography (NR) is the ideal technique for in situ investigations in order to directly observe the hydrogenation behaviour of the metal hydride material inside the tank under operating conditions. Already qualitative investigations revealed interesting macroscopic structure changes for the hydorgen absorption [1,2]. In a further step, the full spectrum of available neutron energies at different imaging beamlines was used for a comprehensive quantitative study of scaled up metal hydride materials, including in operando studies as well as tomography studies. The results help for the optimization of metal hydride based hydrogen storage.

[1]*P. K. Pranzas, et al., Advanced Engineering Materials 13 (8) (2011) 730-736 [2]*Bellosta von Colbe, J.M., Int. Journal of Hydrogen Energy 37, 2012

MM 26.2 Tue 12:00 TC 010

Optimization of Tungsten-Steel Joints for Plasma Facing Components in Fusion Reactors — •Simon Heuer[1], Thomas Weber[2], Jiří Matějíček[3], Jochen Linke[2], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Werkstoffstruktur und -eigenschaften, 52425 Jülich, Germany — [3]Institute of Plasma Physics, Academy of Sciences of the Czech Republic, 18200 Prague 8, Czech Republic

Tungsten, joint to a martensitic-ferritic EUROFER97 structure, is a promising plasma facing material composite for fusion reactors. Due to the effect of mismatch in thermo-mechanical properties direct bonding is not feasible. Current research is therefore ongoing on interlayer systems. While the adhesion was already improved by the utilization of a discrete Cu, Ti or V interlayer, that is able to relax stresses by plastic deformation, joints still do not resist the expected load cycles in a fusion reactor. Therefore, alternatives for the interface are needed. This contribution presents research on functionally graded materials (FGM). The particular microstructure of a graded interlayer allows redistributing macro stresses from a discrete interface to a greater volume while avoiding in particular Cu which tends to swell under neutron irradiation. A parameter study on the basis of finite element analysis will be presented as well as first results of several processing routes for FGM that shall be evaluated and benchmarked by mechanical as well as thermal testing.

MM 26.3 Tue 12:15 TC 010

Assembly of magnetic nano-particles close to a solid wall — •apurve saini, vassilios kapaklis, and max wolff — material physics, department of physics and astronomy, uppsala university, uppsala, sweden

Ferro-fluids are liquids with magnetic nano-particles dispersed in a solvent and show a super-paramagnetic behavior. The magnetic moment makes the particles sensitive to magnetic fields. The application of such a field can drive self-assembly and result in e.g. smectic like ordering.

We investigated the adsorption of magnetic nano-particles close to a ferrofluid-SiO2 interface as a function of external magnetic and flow fields. The particles are stabilized by surface coatings, which makes them extremely sensitive to the termination of a solid boundary and mono- or multilayers can form. The surface energy and polarity of the solid boundary is tuned by self-assembled monolayers.

In situ neutron reflectometry and grazing incidence has been utilized to obtain a detailed microscopic picture of this ordering phenomenon. Thus, the equilibrium as well as kinetics of the self-assembly is studied systematically. Both magnetic fields as well as flow facilitate pronounced layering at the interface,revealing a controlled growth of magnetically nanostructured interfaces on the time scales of hours.

MM 26.4 Tue 12:30 TC 010

Memristive behavior of $TiO_{2-\delta}$ rutile phases – an ab-initio based ground-state analysis — •Wolfgang Heckel[1], Michael Wehlau[2], Sascha B. Maisel[1], Thomas Frauenheim[2], Jan M. Knaup[2], and Stefan Müller[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, D-21073 Hamburg — [2]Bremen Center for Computational Materials Science, University of Bremen, D-28359 Bremen

Memristive devices for various technical applications, e. g. electronic analogues to nerve cells for neuromorphic computing[1], attract growing attention. TiO_2 has been shown to serve as a memristive material.[2]

We conducted a comprehensive ab-initio based ground-state search for $TiO_{2-\delta}$ rutile phases in order to identify structural features which lead to the conductive phase of a TiO_2 memristor. A cluster expansion Hamiltonian, fitted to DFT data, enabled us to scan the entire configuration space of the oxygen vacancies. We find that O vacancies tend to form planar arrangements which relax into structures exhibiting metallic behavior. These structures are energetically less favorable, but show an even more pronounced metallic DOS than the Magnéli phases, which do not appear in our calculations due to energy barriers. Our results confirm the relation between vacancy ordering and metallic behavior in reduced oxides.

Supported by DFG, SFB 986, project A4.

[1] Jo, et al., Nano Letters **10**, 1297 (2010).
[2] Strukov, et al., Nature **453**, 80 (2008).

MM 26.5 Tue 12:45 TC 010

Bose Einstein Condensate observed in Koops-GranMat at RT — •Hans W.P. Koops — HaWilKo GmbH, Ober-Ramstadt, Germany

Giant current density is observed at room temperature in Koops-GranMat(R) with Pt- or Au-nanocrystals embedded in a fullerene matrix. The material is built with Focused Electron Beam Induced Processing. A field emission current up to 1mA was observed at 23 V (Au/C) or 70 V (Pt/C). From an emission site of 10 nm in diameter, the current density reaches in both cases $>$ 1.5 GA/cm2. In 2009 Koops explained the apparent electron-conduction with excitonic electron states in crystal surface orbitals which obey the Bohr Eigenvalue conditions for energy states. The electrons in these excitonic surface orbitals states have a wavelength of 2 nm. The excited excitonic states having a perimeter length of 5 lambda overlap and a Bose Einstein Condensate is formed. Here electrons and holes having parallel spins form Bosons, now named Koops-pairs, they occupy one level only, and show coherent electron emission. Mapping the system on a Bose-Hubbard phase-diagram suggests super-fluidity. The estimated critical temperature for Bose-Einstein-Condensation is higher than room temperature(300K).

MM 27: Transport: Nanomechanics (joint session with MM)

Time: Tuesday 14:00–15:45 Location: A 053

MM 27.1 Tue 14:00 A 053

Inductively coupled cavity optomechanics — •P. Schmidt[1,2], M. Pernpeintner[1,2,3], K.F. Wulschner[1,2], S.T.B. Goennenwein[1,3], A. Marx[1], R. Gross[1,2,3], and H. Huebl[1,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

Cavity optomechanics allows to study the light-matter interaction with micro-, meso-, and macroscopic objects offering the possibility to access the quantum mechanical regime in the literal sense [1]. Transferring this approach to the microwave (MW) domain gives rise to the field of cavity electromechanics. Typical electromechanical systems consist of a micro- or nanomechanical resonator coupled capacitively to a superconducting MW resonator.

Here, we present the approach of an inductively coupled electromechanical system. To this end, we implement a dc-SQUID with a vibrational element at the current antinode of a $\lambda/4$ MW resonator. Hereby, the eigenfrequency of the MW resonator becomes tunable. As the vibration of the nano-string changes the SQUID loop area, we expect that the electromechanical coupling becomes flux-tunable.

We present first experimental results obtained from MW transmission spectroscopy in a dilution refrigerator and compare it with our theoretical model. These results indicate an expected tunability of the electromechanical coupling from 0 to 1 kHz.

[1] M. Aspelmeyer *et al.*, Physics Today **65**, 29 (2012).

MM 27.2 Tue 14:15 A 053

Circuit Electromechanics with a Non-Metallized Nanobeam — •Matthias Pernpeintner[1,2,3], T. Faust[4], F. Hocke[1,2,3], J. P. Kotthaus[4], E. M. Weig[4,5], R. Gross[1,2,3], and H. Huebl[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Nanosystems Initiative Munich, München, Germany — [3]Physik-Department, Technische Universität München, Garching, Germany — [4]Center for NanoScience (CeNS) and Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany — [5]Department of Physics, University of Konstanz, Konstanz, Germany

In the field of cavity optomechanics, a motional degree of freedom is coupled to an optical cavity. This approach can be transferred to the solid state environment e. g. by combining a superconducting microwave cavity with a nanomechanical resonator.

Whereas typically metallized mechanical resonators are used, we present an alternative approach which is based on the dielectric coupling between a superconducting coplanar waveguide microwave resonator and a non-metallized tensile-stressed silicon nitride nanobeam.

We use the Duffing nonlinearity of the strongly driven beam to calibrate the amplitude spectrum of the mechanical motion and determine the electromechanical vacuum coupling. We find a quality factor of 480,000 at a resonance frequency of 14 MHz and 0.5 K. We deduce a vacuum coupling of 11.5 mHz, which is in quantitative agreement with finite element based model calculations.

This type of hybrid platform will allow further studies on the properties of non-metallized beams and more complex mechanical hybrids.

MM 27.3 Tue 14:30 A 053

Coupling Graphene Mechanical Resonators to Superconducting Microwave Cavities — •Peter Weber, Johannes Güttinger, Ioannis Tsioutsios, Darrick E. Chang, and Adrian Bachtold — ICFO-Institut de Ciencies Fotoniques, 08660 Castelldefels (Barcelona), Spain

Graphene is an attractive material for nanomechanical devices because it allows for exceptional properties, such as high frequencies, quality factors, and low mass. An outstanding challenge, however, has been to obtain large coupling between the motion and external systems for efficient readout and manipulation. Here, we report on a novel approach, in which we capacitively couple a high-Q graphene mechanical resonator (Q = 100.000) to a superconducting microwave cavity. The initial devices exhibit a large single-photon coupling of ~10 Hz. Remarkably, we can electrostatically change the graphene equilibrium position and thereby tune the single photon coupling and the mechanical resonance frequency by a large amount. The strong tunability opens up new possibilities, such as the tuning of the optomechanical coupling strength on a time scale faster than the inverse of the cavity line width. With realistic improvements, it should be possible to enter the regime of quantum optomechanics.

MM 27.4 Tue 14:45 A 053

Spin-vibration interaction in a nanomechanical spin-valve — •Pascal Stadler[1], Wolfgang Belzig[1], and Gianluca Rastelli[1,2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Zukunftskolleg, Fachbereich Physik, Universität Konstanz, 78457, Konstanz, Germany

We study spin-dependent transport in a suspended carbon nanotube quantum dot in contact with two ferromagnetic leads and with the dot's spin interacting with the flexural modes [1,2]. The spin-vibration interaction arises from the spin-orbit coupling or a magnetic field gradient. We use a nonequilibrium Green's functions technique to evaluate the phonon occupation and the transport properties. The interaction between the spin and the vibration leads to a mechanical damping and, for an applied bias-voltage, to a steady nonequilibrium occupation of the harmonic oscillator. Depending on the magnetic configuration and the bias voltage polarity, a single vibrational mode can be strongly cooled, heated or can approach a regime of a mechanical instability. Owing to the sensitivity of the electron transport to the spin orientation, we find signatures of the nanomechanical motion in the current-voltage characteristic.

[1] P. Stadler, W. Belzig, and G. Rastelli,
Phys. Rev. Lett. **113**, 047201 (2014).
[2] P. Stadler, W. Belzig, and G. Rastelli, arXiv:1408:6357.

MM 27.5 Tue 15:00 A 053

Large current noise in nanoelectromechanical systems close to continuous mechanical instabilities — Jochen Brüggemann[1], •Guillaume Weick[2], Fabio Pistolesi[3], and Felix von Oppen[4] — [1]I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [2]Institut de Physique et Chimie des Materiaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, F-67034 Strasbourg, France — [3]Laboratoire Ondes et Matiere dÁquitaine, Université de Bordeaux, CNRS UMR 5798, F-33400 Talence, France — [4]Dahlem Center for Complex Quantum Systems & Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany

We investigate the current noise of nanoelectromechanical systems close to a continuous mechanical instability. In the vicinity of the latter, the vibrational frequency of the nanomechanical system vanishes, rendering the system very sensitive to charge fluctuations and, hence, resulting in very large (super-Poissonian) current noise. Specifically, we consider a suspended single-electron transistor close to the Euler buckling instability [1,2,3]. We show that such a system exhibits an exponential enhancement of the current noise when approaching the Euler instability which we explain in terms of telegraph noise [4].

[1] G. Weick et al., PRB 81, 121409(R) (2010)
[2] G. Weick et al., PRB 83, 035420 (2011)
[3] G. Weick et al., PRB 84, 125454 (2011)
[4] J. Brüggemann et al., PRB 85, 125441 (2012)

MM 27.6 Tue 15:15 A 053

Mechanically induced iSWAP gate and maximally entangled states in a carbon nanotube — •Heng Wang and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study a nanomechanical system where two separated single-electron spins in two quantum dots in a suspended carbon nanotube (CNT) are driven by an ac electric field in a parallel magnetic field. An indirect coupling between two single-electron spins is induced based on the simultaneous interaction of the two spins with the mechanical mode of the CNT. We show how a two-qubit iSWAP gate and arbitrary single-qubit gate can be obtained by analyzing the effective Hamiltonian from the time dependent Schrieffer-Wolff transformation and the time evolution operator. Combining the iSWAP gate and single-qubit gates, maximally entangled states of two spins can be generated with a single step by varying the frequency and the strength of the external electric driving field. The iSWAP gate and single-qubit gates can be turned off when suppressing the spin-phonon coupling by electrostatically shifting the electron wave function on the nanotube.

MM 27.7 Tue 15:30 A 053

Nonlinear phononics using atomically thin membranes — Daniel Midtvedt and •Alexander Croy — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

In recent years, there has been considerable interest in tailoring material and wave-propagation properties using structured materials, prominent examples being phononic and photonic crystals. Here, we propose a design that allows for engineering flexural-phonon propagation by facilitating atomically thin membranes [1]. The strong geometric nonlinearity present in such systems leads to phonon-phonon interactions, which allow the study of many-body effects. Using a continuum mechanics description of a periodically pinned graphene membrane, we investigate the properties of the resulting phononic crystal and demonstrate that defects in the pinning lattice support localized modes. Two such modes in close proximity interact via the elastic energy, and constitute a simple model of a phononic dimer. We show that the defect Hamiltonian in the rotating-wave approximation is equivalent to a classical Bose-Hubbard model. By tuning the properties of the pinning lattice and the amplitudes of the flexural vibrations, we observe a bifurcation corresponding to the transition from "Rabi" to "Josephson" dynamics. Further, we demonstrate a wide tunability of the dimer frequencies by local back-gates, which allows for studies of the (non-linear) Landau-Zener transition.

[1] D. Midtvedt, A. Isacsson and A. Croy, Nat. Commun. **5**, 4838 (2014).

MM 28: Poster Session II

Time: Tuesday 18:30–20:30 Location: Poster E

MM 28.1 Tue 18:30 Poster E

Molecular dynamics simulation of mechanical properties of dilute α-Fe-C alloys — •Jan Janssen, Nina Gunkelmann, and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

Using molecular dynamics simulation, we study the influence of carbon interstitials on the mechanical properties of α-iron. With increasing carbon concentration we observe an increase of the tetragonal distortion and a decrease of the elastic moduli. Furthermore we analyze various available iron-carbon potentials and compare the results to ab-initio calculations and experimental data.

MM 28.2 Tue 18:30 Poster E

Fitting an Interatomic Potential for Accurate Description of the Iron-Chromium System — •Sebastian Eich, Daniel Beinke, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, D-70569 Stuttgart, Germany

A new potential for the iron-chromium (Fe-Cr) system was developed using the formalism of the embedded-atom method (EAM) within the two-band model (TBM) extension. The key improvement of this potential in comparison to available ones from literature is the accurate description of the miscibility gap according to experimental data and a recent CALPHAD parametrization. Furthermore, the potential was fitted to obtain an enriched solubility of chromium atoms in an iron matrix at 0 K which is predicted by several ab-initio calculations. The potential was also benchmarked against phonon excess entropies at 300 K and 1600 K and shows good agreement with inelastic neutron scattering measurements.

The development was restricted to the metastable α/α' phase and for the fitting only the direct interaction between iron and chromium was taken into account while the potentials for pure elements were taken from literature (Ackland[1] (Fe) and Olsson[2] (Cr)).

[1] Ackland et al., J. Phys.: Condens. Matter 16, S2629 (2004)
[2] Olsson et al., Phys. Rev. B 72, 214119 (2005)

MM 28.3 Tue 18:30 Poster E

Calculation of Electronic Thermophysical Parameters for Steel Alloys based on Density Functional Theory — •Juergen Sotrop[1], Jan Winter[1], Heinz P. Huber[1], Stephan Borek[2], and Jan Minar[2,3] — [1]Munich University of Applied Sciences — [2]Ludwig-Maximilians Universit, Muenchen — [3]University of West Bohemia, Pilsen

The ablation mechanism of matter irradiated with ultra-short laser pulses has been widely investigated over the last two decades. At present there is still lack of theoretical understanding of the interaction of ultra-short laser pulses with a metal alloy. By irradiating material with ultra-short laser pulses initially strong electron-phonon nonequilibrium will occur. The resulting difference in electron and phonon temperatures can be calculated with the so called two-temperature model (TTM). An essential prerequisite for the application of the TTM is a determination of the temperature dependent thermophysical parameters such as electron heat capacity and electron-phonon coupling factor. We will present a general method for the calculation of the electronic thermophysical parameters for metal alloys, here performed exemplarily on stainless steel (AISI 304). The method is based on the calculation of the electronic density of states (DOS) using a fully relativistic implementation of the KKR-formalism in the framework of spin density functional theory. Precise knowledge of the DOS will enable the calculation of the electron-phonon-coupling factor and the electron heat capacity. The model is compared with the well-known parameters for iron to show the validity.

MM 28.4 Tue 18:30 Poster E

Exact models and numerics for the relativistic single-site scattering problem — •Matthias Geilhufe[1], Steven Achilles[2], Markus Arthur Koebis[3], Martin Arnold[3], Ingrid Mertig[2,1], Wolfram Hergert[2], and Arthur Ernst[4,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [3]Institut für Mathematik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [4]Wilhelm-Ostwald-Institut für Physikalishe und Theoretishe Chemie, Universität Leipzig, Leipzig, Germany

The Korringa-Kohn-Rostoker Green function method (KKR) based on density functional theory is a powerful tool for electronic structure calculations. For the discussion of spin-orbit coupling driven phenomena e.g. on surfaces a fully-relativistic treatment within the full-potential approximation [1] is necessary. The numerical solution of the fully relativistic single-site scattering will be discussed for the Coulomb and the Mathieu potential. In this context, the solution of the fully-relativistic full-potential single-site scattering problem using integral equations is compared with a direct solution of the differential equations via various methods. The advantages and disadvantages of the used methods will be discussed and proposals for accurate and efficient methods will be given.

[1] T. Huhne et al., PRB **58**, 16, 10236 (1998)

MM 28.5 Tue 18:30 Poster E

Correlation energy evaluation in extended systems beyond the RPA — •Emanuele Maggio and Georg Kresse — University of Vienna, Faculty of Physics and Centre for Computational Materials Science, Sensengasse 8/12, Vienna, Austria

The description of electronic correlations plays a pivotal role in the accurate modelling of structural and electronic properties of materials [1]. A range of well-developed methods has come into maturity in recent years [2, 3]; however a full scale assessment of the correlation energy remains restricted to systems with very few atoms per unit cell owing to the high computational demands.

To improve upon the Random Phase Approximation (RPA), we develop a computational scheme that exactly includes all second order contributions [4, 5] to the correlation energy and is also able to implicitly account for higher order diagrams. The inclusion of an effective screened interaction between electrons, alongside an improved description of the reference state at the GW_0 level of theory are key features of the method proposed, whose performance is assessed for a set of prototypical semiconducting materials and for the homogeneous electron gas.

[1] Harl, J.; Schimka, L.; Kresse, G. *Phys. Rev. B* **2010**, 81, 115126. [2] Shepherd, J. J.; Booth, G. H.; Alavi, A. *J. Chem. Phys.* **2012**, 136, 244101. [3] Booth, G. H.; Grüneis, A.; Kresse, G.; Alavi, A. *Nature* **2013**, 493, 365-370. [4] Bates, J. E.; Furche, F. *J. Chem. Phys.*

2013, 139, 171103. [5] Grüneis, A.; Marsman, M.; Harl, J.; Schimka, L.; Kresse, G. *J. Chem. Phys.* **2009**, 131, 154115.

MM 28.6 Tue 18:30 Poster E

Gutzwiller Density Functional Theory — •Tobias Schickling, Jörg Bünemann, and Florian Gebhard — FB Physik, Philipps Universität Marburg, D-35032 Marburg, Germany

Density Functional Theory (DFT) is the workhorse of electron structure theory. It reduces the genuine many-body problem to an effective single-particle theory that is readily evaluated numerically. However, electrons in narrow bands, e.g., 3*d*-electrons in transition metals and their compounds, require a more sophisticated treatment. Unfortunately, model Hamiltonians for correlated electrons often oversimplify the problem while, at the same time, they reintroduce the full complexity of the many-body problem. I present the Gutzwiller DFT that combines the advantages of both schemes: it retains the computational efficiency of existing DFT codes and it treats electronic correlations on the basis of Gutzwiller's variational many-body approach for multiband Hubbard models. A first application to fcc nickel resolves all of the DFT shortcomings regarding lattice spacing, magnetic moment, bulk modulus, and Fermi-surface topology. Moreover, I will show results of the bcc-hcp transition of iron.

MM 28.7 Tue 18:30 Poster E

Automatically generated MEAM potentials from DFT for simulation of Li_xSi_y battery materials — •Sebastian Schwalbe and Jens Kortus — TU Freiberg, Institute of Theoretical Physics

We implemented an optimization procedure using the so called particle swarm optimization (PSO [1]) to automatically optimize modified embedded atom method (MEAM [2,3]) parameters. In detail physical properties (elastic constants, bulk modulus, total energy) calculated with density functional theory (DFT) will be used as constraints for the PSO algorithm leading to a DFT like accuracy MEAM potential. We generated these optimized MEAM potentials for Li and Si to be used for large scale simulations of Li_xSi_y battery materials.

[1] J. Kennedy, R. Eberhart, IEEE Vol. 4 (1995), pp. 1942-1948
[2] Murray S. Daw, and M. I. Baskes, Phys. Rev. B 29(12), 1984.
[3] B. Jelinek, S. Groh et al., Phys. Rev. B 85(24), 2012.

MM 28.8 Tue 18:30 Poster E

Efficient numerical treatment of irregular coupled radial scattering solutions — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The numerical determination of the coupled radial scattering solutions of the stationary Schrödinger equation for a general non-spherical potential is particularly difficult if one needs not only the regular but also the irregular solutions. These are, for instance, necessary in the complex energy formulation of the Korringa-Kohn-Rostoker (KKR) Green-function (GF) method. The difficulty for the irregular solutions arises from their divergent behaviour near the origin where functions of very different magnitudes are coupled. A technique will be presented which overcomes this problem by use of an analytical decoupling scheme and a subinterval procedure with Chebyshev interpolations in each subinterval. It will be shown that accurate irregular solutions can be obtained and that this is important for the calculation of precise forces in the KKR-GF method.

MM 28.9 Tue 18:30 Poster E

Computational Study of Cu Doped Ag Nano Alloy Clusters. — •Prabhat Ranjan — MANIPAL UNIVERSITY JAIPUR, JAIPUR, INDIA.

There is a number of reports available in favour of Bi-metallic nano alloy clusters for a wide range of applications. As the bi-metallic nano alloy clusters have diverse physico-chemical properties, among such nano clusters, the compounds formed between Cu-Ag have gained a considerable interest because they possess unique optical, electronic and magnetic and mechanical properties, which have extensive applications in the field of optoelectronics, optics and nanoscience. Density Functional Theory (DFT) is one of the most popular techniques of quantum mechanics to study the electronic properties of materials. Recently, conceptual DFT based descriptors have been turned to be indispensable tools for studying the experimental properties of compounds. In this work we reported a theoretical analysis on the stabilities, electronic properties and geometries of Cu-Agn; (n=1-10) system using B3LYP with basis set LanL2DZ. The electronic properties of Cu-Agn Viz. HOMO-LUMO gap (eV), Global Hardness (η), Global Softness (S), Electronegativity(χ), Electrophilicity Index(ω), Dipole Moment and Bond length are successfully computed and compared in terms of DFT based global descriptors. This study is probably the first attempt to explore the electronic properties of Cu-Agn Nanoalloy cluster in terms of DFT based descriptors.

MM 28.10 Tue 18:30 Poster E

Calculated Mechanical and Thermal Properties of $CePt_3Si$ and $CePt_3B$ above their Magnetic-Ordering Temperatures by an LDA-Based Ab-Initio Theory — •Rudolf Sykora[1], Dominik Legut[2], Gerda Rogl[3,4,5], Peter Müller[4], Herbert Müller[4], Ernst Bauer[4], Stephan Puchegger[5], and Peter Rogl[3] — [1]Nanotechnology Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [3]Institute of Physical Chemistry, University of Vienna, Wien, Austria — [4]Institute of Solid State Physics, University of Technology, Wien, Austria — [5]Faculty of Physics, University of Vienna, Wien, Austria

Adopting the plane-wave pseudopotential VASP[1] DFT package, using a simple local density approximation for electronic exchange and correlation effects, and disregarding spin-orbit interaction we calculate (a necessarily naive) electronic structure of $CePt_3Si$ and $CePt_3B$ materials (the former being known as a heavy-fermion superconductor with no inversion centre) under several discrete values of stress and strain. For each such configuration we calculate its phonon spectrum with a direct (supercell) method as supplied by the Phonopy program. Combining the results we obtain materials' thermal and mechanical properties within the quasi-harmonic approximation, presumably applicable to temperatures above magnetic-ordering temperatures. Results are compared to experimental data.

References:

1.G. Kresse, J. Furthmueller, J. Comput. Mater. Sci. **6**, 15 (1996).

MM 28.11 Tue 18:30 Poster E

Simulation of the elastic properties of nanomechanical beam and membrane resonators — •Kristian Scholz, Ananta Käl-berer, Tobias Kemmer, Thomas Möller, Daniel Mutter, Markus Ring, Ralf Schmid, Martin Vögele, and Peter Nielaba — University of Konstanz, Germany

The oscillation behavior of nanomechanical resonators in the form of doubly clamped beams and clamped membranes is investigated by Molecular Dynamics simulations. After setting up the initial structure, the end points of the beams or the outer border of the membranes, respectively, are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the structures. Besides varying the size of the structures, the effects of temperature, external stretching fields, cavities and crystal faults are explored. The results show a decrease of the oscillation frequencies and an increase of the damping coefficient with rising temperature, a strong increase of the frequencies with external stress (stretching), a decrease of frequencies with size and an increase of the damping coefficient when adding cavities to the structures. It is also possible to observe the dissipation of energy from the collective oscillation of the structures into thermal energy of the degrees of freedom of the constituting atoms.
Different materials (e.g. Si, Si_3N_4 and NiTi memory alloys) are explored as well. In order to explore quantum effects in the low temperature regime Path Integral Monte Carlo simulations are performed.

MM 28.12 Tue 18:30 Poster E

Nanoporous Germanium-Silicon alloys by ion irradiation at low energies — •Fritz Lehnert[1] and Stefan G. Mayr[1,2,3] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM) — [2]ranslationszentrum für regenerative Medizin (TRM) Leipzig — [3]Fakultät für Physik und Geowissenschaften, Universität Leipzig

Nanoporous materials exhibit a very large surface area compared to their volume and are therefore an interesting material class for all surface active processes such as catalysis membranes or gas adsorption storage applications. While the influence of ion radiation on single-crystal germanium as a semiconductor material, has been studied in the past decades, the effects on their alloys remains yet uninvestigated. Therefore the development of a nanoporous surface layer during ion bombardment of germanium-silicon-alloys was studied in detail experimentally. Amorphous germanium-silicon thin films produced by electron beam evaporation were irradiated with low energy 30 keV Ga-ions using a focued ion beam. The surface morphology and topography was investigated by SEM and AFM measurements. The nano-structure de-

velopment was found to depend strongly on the silicon-to-germanium ratio. The investigation of semiconductor alloys is expected to lead to a better understanding of the processes involved in the development of a nanoporous structure by ion bombardment.

[1] S. G. Mayr and R. S. Averback, Phys. Rev. B 71 (2005) 134102.

MM 28.13 Tue 18:30 Poster E

Absolute Photoluminescence Quantum Yields and Lifetimes of in Toluene Dispersed Hexagonal β-NaYF$_4$: x % Tm^{3+}, 20 % Yb^{3+} Upconversion Nanoparticles — •Marco Kraft[1], Martin Kaiser[1], Christian Würth[1], Tero Soukka[2], and Ute Resch-Genger[1] — [1]BAM Bundesanstalt für Materialforschung und -prüfung, Richard-Willstaetter-Str. 11, 12489 Berlin — [2]Department of Biotechnology, University of Turku, Tykistoekatu 6A, FI-20520 Turku, Finland

Hexagonal β-NaYF$_4$ doped with Yb^{3+} and Tm^{3+} is an efficient upconversion (UC) phosphor for the conversion of 976 nm to 800 nm and 450 nm light. The emission behavior of this material is strongly influenced by the doping concentration, particle size, and surface chemistry. The design of nm-sized UC particles requires reliable spectroscopic tools for the characterization of the optical properties of these materials like the UC quantum yield (QY_{UC}). This UC emission originates from multiphotonic absorption processes, rendering the QY_{UC} excitation power density (P) dependent. The absolute measurement of QY_{UC} presents a considerable challenge due to the low absorption coefficient and the P-dependence of these materials, which can introduce a dependence of QY_{UC} on illumination geometry. Here, we present the P-dependent QY_{UC} of 30 nm-sized NaYF$_4$ UC particles with systematically varied dopant concentrations of 20 % Yb^{3+} and x % Tm^{3+} (x = 0.2, 0.5, 0.8, 1.1, 2). In addition to QY$_{UC}$, the emission intensities and lifetimes of the different UC bands are studied as function of excitation power density to gain a better insight of their photonic nature.

MM 28.14 Tue 18:30 Poster E

Structural and electronic properties of amorphous graphene — •Soumyajyoti Haldar[1], Basu Oli[2], Parthapratim Biswas[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Department of Physics and Astronomy, University of Southern Mississippi, USA

Non-crystalline graphene structures have interesting structural and electronic aspects, which may be explored for various applications. In our work, amorphous graphene in various number densities (lower and higher compared to crystalline graphene) and system sizes ($\sim$ 500-2048/supercell) have been simulated using density functional based molecular dynamics and Monte Carlo techniques. The resulting structures have a variety of networks of disordered small and large carbon rings, which have been analyzed by ring and Mermin statistics. Interestingly, linear chains of carbon atoms are also observed for certain densities. Comparisons have been made with recent experimental and theoretical studies[1,2]. Our calculations of densities of states show finite contributions at the Fermi level. The analysis of inverse participation ratio confirms that the states near the Fermi energy are delocalized.

Reference:
1. E. Holmström, J. Fransson, O. Eriksson et. al. Phys. Rev. B 84, 205414 (2011)
2. F. Eder, J. Kotakoski, U. Kaiser et. al. Scientific Reports 4, 4060 (2014)

MM 28.15 Tue 18:30 Poster E

Plasticity at the low end of the nanoscale - a crossover to glass-like behavior? — •Christian Braun, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

Polycrystalline metals at the low end of the nanoscale with grain sizes of 10 nm or less are characterized by a grain boundary volume fraction of at least 30%. Grain boundary deformation modes similar to shear transformations (STs) in bulk metallic glasses (BMGs) may therefore play a non-negligible role in the mechanical behavior of nanocrystalline (nc) metals. In fact, a couple of similarities between this two material classes have been observed, e.g. comparable values for the shear activation volume, activation energy or Mohr-Coulomb friction coefficient. However, in BMGs increasing load involves percolation of STs followed by shear band formation manifesting stick-slip behavior that eventually leads to catastrophic failure. In contrast, for nc Pd90Au10 we observe absence of stick-slip behavior implying that shear banding is missing. In fact, the operation of STs at/along grain boundaries in conjunction with the network constraints of the nanoscale microstructure avoids pronounced shear band propagation. We present results of mechanical testing of nc Pd90Au10 samples synthesized by inert gas condensation and deformed in shear compression geometry under different loading conditions. These results are analyzed in terms of activation parameters and pressure or normal-stress dependence of plasticity. Furthermore, the interplay and the succession of active deformation mechanisms are investigated using in situ X-ray diffraction.

MM 28.16 Tue 18:30 Poster E

Investigation of the magnetic phase transition in iron-rhodium thin films by ferromagnetic resonance — •Alirerza Heidarian[1], Jürgen Lindner[1], Rantej Bali[1], Kay Potzger[1], Jörg Grenzer[1], Sven Hoffmann[1], Michael Farle[2], and Florian Römer[2] — [1]HZDR Institute of Ion-Beam Physics and Materials Research, Dresden, Germany — [2]Faculty of Physics and Center for Nanointegration, University of Duisburg-Essen, Duisburg, Germany

Due to the first-order phase transition from an antiferromagnetic (AF) to a ferromagnetic (F) state at 370 K, the equiatomic FeRh alloy has raised growing interest. In our study, the phase transition of FeRh thin films was analyzed by means of ferromagnetic resonance (FMR). $Fe_{50}Rh_{50}$ films are obtained by molecular beam epitaxy on MgO single-crystal substrates. The films are 37 nm and 6 nm thick and were co-deposited from separate Fe and Rh sources. FMR was observed in an X-band cavity set-up, with variable temperature. As the temperature crosses 370 K, resonance lines associated with the F phase appear. Furthermore, resonance lines due to possible acoustic- and optical-resonance modes are observed. Our measurements show that temperature dependent FMR can be used to determine the relative volumes of AFM and FM regions across phase transition. The transition from AF to F coupling can therefore be tracked using FMR measurements. Moreover, the phase transition temperature for 6 nm thick film is 285 K which resonance lines of F phase emerge. Therefore FMR can be an effective tool in unraveling coupling phenomena in FeRh.

MM 28.17 Tue 18:30 Poster E

Laser assisted fabrication of chalcogenide nanostructures with tailored morphology — •Thomas Vasileiadis[1,2] and Spyros N. Yannopoulos[1] — [1]Foundation for Research and Technology Hellas, Institute of Chemical Engineering Sciences (FROTH/ICE-HT), P.O. Box 1414, GR-26504, Rio-Patras, Greece — [2]Fritz Haber Institut der Max Planck Gesellschaft, Faradayweg 4 - 6, D - 14195 Berlin, Germany

Low dimensional nanostructures of chalcogens and chalcogenides have attracted considerable attention over the last years. Here we present a simple and cost effective laser-assisted method for the growth of low dimensional nanostructures based on functional chalcogenides. Te nanotubes can be easily prepared via cw laser ablation in a one-step method. By changing the irradiation conditions different morphologies arise in a controllable way, such as t-Te nanospheres. Differences in the morphology control are observed for elemental Se, a good glass-former. This synthetic strategy can be readily applied in many other functional chalcogenides e.g. As2S3 and phase-change materials, e.g. GeTe. Since chalcogenides are mostly famous for their sensitivity to external stimuli such as light, post-treatment of the resulting nanostructures with low light fluence is also investigated. A series of light-driven phase transition is employed to controllably transform Te nanotubes to core-Te/sheath-TeO2 and/or even neat TeO2 nanowires.

MM 28.18 Tue 18:30 Poster E

metallic nanoparticles and nanoalloys fabricated via solid state deweting — •Dong Wang, Andreas Herz, and Peter Schaaf — TU Ilmenau, FG Werkstoffe der Elektrotechnik, Ilmenau, Germany

metallic an alloy nanoparticles are paid increased attention due to their potential applications in catalysis, magnet memories, sensors, and plasmonics. Here, nanoparticles, nanoporous nanoparticles and bi-metallic nanoparticles were fabricated by using solid-state dewetting. By using pre-patterned substrate, ordered arrays of nanoparticles can be realized due to the curvature driven diffusion through the modulation of the chemical potential by substrate local curvature. By combining the solid state dewetting of Ag/Au bilayer with a subsequent dealloying process, nanoporous gold nanoparticles were fabricated, and possess a different plasmonic property comparing to the solid gold nanoparticles. In addition, the alloying behavior in the microscale can be well studied through the solid state dewetting of metallic bilayer. Different Ni-Au nanoparticles were realized by controling the process parameters.

MM 28.19 Tue 18:30 Poster E

In-situ and ex-situ HRTEM characterization of heated, supersaturated metal-carbide nanoparticles — •Michael Hering[1,2], Darius Pohl[1], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]TU Dresden, IFWW, D-01062 Dresden, Germany

The segregation of carbon from supersaturated metal-carbon compounds is a highly important step in the production of many novel materials. It is, e. g., an essential process during the growth of carbon nanotubes or in the formation of high-anisotropy granular magnetic FePt-X films. A detailed knowledge of this segregation is thus mandatory. Inert gas condensation is utilized to fabricate Fe-C and Ni-C nanoparticles, and much effort is made to determine the key parameters to tune the size, morphology and structure of the particles in order to generate single-crystalline or well faceted polycrystalline carbide particles with high carbon content. The characterization of these particles is then performed in an aberration-corrected FEI Titan^3 80-300 microscope. The poster presents in a first part the different types of Fe-C and Ni-C particles and correlates the observed structures to the applied process parameters. E.g., in case of Fe-C nanoparticles, the inert gas condensation process mostly results in the formation of particles with a distinct core-shell structure of an iron core surrounded by a carbide shell. The carbon segregation of these particles as induced by a thermal treatment is then presented in the second part. Therefore, a special TEM sample holder for in-situ heating experiments with silicon nitride window chips is used.

MM 28.20 Tue 18:30 Poster E

Highly ordered one-dimensional metal nanowire arrays for SERS — •yong-tae kim[1], stefan l. schweizer[1], jörg schilling[1], and ralf b. wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg, Halle, Germany — [2]Fraunhofer Institute for Mechanics of Materials, Halle, Germany

Recent progress in nanotechnology have created new insight about controlling various structures and properties of nanostructured materials that can support surface plasmons for specific applications. Especially metallic nanostructured materials made of noble metals show localized surface plasmon resonance (LSPR) phenomenon when the materials interact with incident light of correct frequency and polarization.

Surface-enhanced Raman spectroscopy (SERS) has been recognized as a useful tool for ultra-sensitive detection of trace amount of chemicals with fingerprint character. The SERS intensity depend strongly on the electromagnetic field enhancement induced from LSPR at nanogaps between plasmonic nanostructures, called hot spots. To obtain high sensitivity and good reproducibility of SERS signal, it is required to have a highly ordered nanostructures with well-controlled narrow gaps that induce hot spots.

Herein, highly ordered one-dimensional metal nanowire arrays with single- or multi-segmental structures composed of gold, silver, and nickel have been prepared via hard-template synthetic method as an active substrate for SERS. Those materials have been investigated to study the effect of dimension and composition of metal nanowire arrays on SERS enhancement factor.

MM 28.21 Tue 18:30 Poster E

Simulation of Nanocolumn Formation in a Plasma Environment — •Jan Willem Abraham[1], Thomas Strunskus[2], Franz Faupel[2], and Michael Bonitz[1] — [1]Institut für Theoretische Physik und Astrophysik, CAU Kiel — [2]Institut für Materialwissenschaft, CAU Kiel

Recent experiments and kinetic Monte Carlo (KMC) simulations [1,2] demonstrated that physical vapor co-deposition of a metal alloy (Fe-Ni-Co) and a polymer (Teflon AF) can lead to self-organized growth of magnetic nanocolumns. While these experiments have been carried out with thermal sources, we analyze the feasibility of this process for the case of a sputtering source. For that purpose, we extend our previous simulation model by including a process that takes into account the influence of ions impinging on the substrate [3]. The simulation results predict that metal nanocolumn formation should be possible. Furthermore we show that the effect of ions, which create trapping sites for the metal particles, is an increased number of nanocolumns.

[1] H. Greve et al., Appl. Phys. Lett. 88, 123103 (2006)
[2] L. Rosenthal et al., J. Appl. Phys. 114, 044305 (2013)
[3] J.W. Abraham et al., submitted to J. Appl. Phys. (2014)

MM 28.22 Tue 18:30 Poster E

Polar Catastrophy by Incremental Charge Differences — •Arwa Abdullah Albar — King Abdullah University of Science and Technology, Thuwal , Saudi Arabia

We report the creation of a two-dimensional electron gas at the SnO/SnO_2 heterointerface. To analyze the mechanism behind this observation, we study the electronic states as a function of the distance to the interface. A polar catastrophy scenario based on incremental charge differences due to covalency effects is developed to explain the creation of the electron gas. This scenario applies not only to polar/polar interfaces but also modifies the expected carrier density at polar/nonpolar interfaces of semiconducting perovsite oxides, in agreement with experimental results.

Authors: A. Albar, H. A. Tahini and U. Schwingenschlögl
Affiliation: Physical Science and Engineering division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia

MM 28.23 Tue 18:30 Poster E

Atomistic simulations of interfaces and dislocations in Mg-Al alloys — •Tobias Klöffel[1,2], Bernd Meyer[2], and Erik Bitzek[1] — [1]Materials Science and Engineering, Institute I, FAU Erlangen-Nürnberg — [2]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Their low density and high strength make magnesium alloys key structural materials for lightweight constructions. The intermetallic $Mg_{17}Al_{12}$ phase is the dominant precipitate phase and influences to a large degree the mechanical properties of Mg alloys. Here we present a computational study of $Mg/Mg_{17}Al_{12}$ interphase boundaries (IPBs), combining density functional theory (DFT) calculations with large-scale atomistic simulations using a semi-empirical potential of the modified embedded atom method (MEAM) type. DFT calculations of the γ surfaces in $Mg_{17}Al_{12}$ are used to validate the MEAM potential. DFT and atomistic calculations were then performed to characterize the IPB structure and energy for different orientation relationships to the Mg matrix. The results are compared to both, theoretical and experimental findings. Additional atomistic simulations were performed to determine the core structure and Peierls stress of various dislocations in the $Mg_{17}Al_{12}$ phase.

MM 28.24 Tue 18:30 Poster E

Measuring the Stress Distribution of Bio-Inspired Adhesives in Contact — •Jens W. Neubauer[1], Longjian Xue[2], Johann Erath[1], Dirk-Michael Drotlef[2], Aránzazu del Campo[2], and Andreas Fery[1] — [1]Physikalische Chemie II, Universität Bayreuth, Bayreuth, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

The responsiveness and the strong restoring forces of polyelectrolyte brushes can be utilized to sense stresses on the microscale. Therefore, a polycationic brush was labeled with a fluorescent dye allowing to measure local pressures as low as 10 kPa from the mechano-response with a lateral resolution better than human skin (1 μm).

Applying a defined pressure with soft colloidal probe AFM, the fluorescence was observed with a confocal microscope. After calibration, the pressure distribution under bio-inspired microstructured adhesives in contact could be determined from the fluorescence of the polymer brush. The contact formation of the adhesives was controlled with a commercial setup (PVM-A, GeSiM).

Furthermore, the steric interactions of the polyelectrolyte brush were investigated. By force-mapping a pattern with brush-free areas, the separation on the polyelectrolyte brush could be defined without reaching the constant compliance regime.

MM 28.25 Tue 18:30 Poster E

Characterization of bioinspired hybrid materials by multi-scale analysis — •Britta Seidt[1], André Gjardy[1], Keith Gregorzyk[2], Mato Knez[2], Valeria Samsoninkova[3], Felix Hansske[3], Hans Börner[3], Peter Fratzl[1], and Wolfgang Wagermaier[1] — [1]Max Planck Institute of Colloids and Interfaces, Germany — [2]CIC nanoGune Consolider, Spain — [3]Humboldt-Universität zu Berlin, Germany

Specially designed hybrid materials can be used as a model system to compare its properties and structural design principles with those of biological materials such as bone. We aim to develop new combinations of multi scale analytic tools, to investigate the correlation between macroscopic material mechanics and microscopic structure of bioinspired hybrid materials. To understand deformation processes in two model systems, X-ray scattering techniques and tensile testing ex-

periments were combined in a specially designed apparatus. The first model system is a composite material, composed of submicron metal fluoride particles embedded in a poly(ethylene oxide) matrix. First results allow us to follow crystal orientation effects during tensile testing, indicating a reorientation of crystalline domains in the material. The second model system is based on natural collagen extracted from turkey leg tendons as organic part infiltrated with different metals. We investigated the usability of these tendons as matrices for metal infiltration and compared untreated collagen with metal-infiltrated collagen. First results lead us to the assumption of a directional embedding of the metals into the collagen structure.

MM 28.26 Tue 18:30 Poster E

Characteristics of the artificial nanocrystalline calcium carbonate microlens arrays subjected to the amorphous/crystalline phase transformation — •Ingo Schmidt[1], Kyubock Lee[2], Emil Zolotoyabko[3], Peter Werner[4], Peter Fratzl[1], and Wolfgang Wagermaier[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Korea Institute of Energy Research, Daejeon, Korea — [3]Technion - Israel Institute of Technology, Haifa, Israel — [4]Max Planck Institute of Microstructure Physics, Halle, Germany

Natural biogenic materials with extraordinary properties, which often reveal a hierarchical arrangement of simple building blocks, serve as a comprehensive source for bio-inspired synthetic materials. Here we present structural aspects of nanocrystalline bioinspired calcite microlens arrays fabricated via an amorphous pre-phase. By the aid of polarized light microscopy we show that the calcite MLA crystallizes in spherulite-like patterns without changing the shape of individual microlenses. By mapping the local mean crystal orientations by microfocus X-ray diffraction, we find that the crystallization front propagates radially from the nucleation event, with the c-axis of calcite being the crystal growth direction. TEM observations indicate an average calcite crystal size of about 15-20 nm. Such nanocrystallites minimize birefringent effects and inhibit undesirable light scattering at grain boundaries. The knowledge of the MLA crystallization pathways may give us new information on biomineralization processes in calcite-based bio-composites.

MM 28.27 Tue 18:30 Poster E

Hydrophobic interaction governs unspecific adhesion of staphylococci: a single cell force spectroscopy study — •Nicolas Thewes[1], Peter Loskill[1], Philipp Jung[2], Henrik Peisker[2], Markus Bischoff[2], Mathias Herrmann[2], and Karin Jacobs[1] — [1]Saarland University, Saarbrücken, Germany — [2]Saarland University Hospital, Homburg/Saar, Germany

Unspecific adhesion of bacteria is usually the first step of biofilm formation on abiotic surfaces, yet it is unclear up to now which forces are governing this process. Alongside long-ranged van der Waals and electrostatic forces, short-ranged hydrophobic interaction plays an important role. To characterize the forces involved during approach and retraction of an individual bacterium to and from a surface, single cell force spectroscopy is applied: A single cell of the apathogenic species S. carnosus isolate TM300 is used as bacterial probe. With the exact same bacterium, hydrophobic and hydrophilic surfaces can be probed and compared. We find that as far as 50 nm from the surface, attractive forces can already be recorded, an indication of the involvement of long-ranged forces. Yet, comparing the surfaces of different surface energy, our results corroborate the model that large, bacterial cell wall proteins are responsible for adhesion, and that their interplay with the short-ranged hydrophobic interaction of the involved surfaces is mainly responsible for adhesion. The ostensibly long range of the attraction is a result of the large size of the cell wall proteins, searching for contact via hydrophobic interaction. The model also explains the strong (weak) adhesion of S. carnosus to hydrophobic (hydrophilic) surfaces.

MM 28.28 Tue 18:30 Poster E

The influence of the stacking fault energy on the microstructure evolution of severely deformed Cu-Ni alloys — •Friederike Emeis, Gerhard Wilde, Harald Rösner, and Matthias Wegner — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, D-48149

Copper and nickel are completely miscible in the liquid and solid state forming face-centered cubic alloys. The microstructure evolution of different compositions (10/90, 50/50 and 90/10) was investigated after severe plastic deformation using high pressure torsion (HPT) followed by annealing. The grain size is thus reduced and the hardness increases. This microstructure evolution is influenced by the stacking fault energy (SFE). The SFE indicates how easily dislocations can form, which are required to operate for an easy plastic flow of the material. Other factors, such as precipitation hardening, can be neglected due to the complete miscibility. The grain size distributions, twin densities, dislocation densities and hardness were characterized using electron backscatter diffraction (EBSD) and Vickers Hardness measurements. The SFEs of the different alloys were experimentally determined by the dissociation width of the present dislocations using transmission electron microscopy (TEM). The obtained results are discussed.

MM 28.29 Tue 18:30 Poster E

Hot Isostatic Pressed Tungsten Fiber-Reinforced Tungsten — •Bruno Jasper[1], Jan W. Coenen[1], Johann Riesch[2], Till Höschen[2], and Christian Linsmeier[1] — [1]Forschungszentrum Juelich GmbH, IEK4 - Plasmaphysik, 52425 Jülich, Germany — [2]Max-Planck-Institut für Plasmaphysik, 85748 Garching, Germany

Tungsten fiber-reinforced tungsten (W_f/W) is a composite material that addresses the brittleness of tungsten (W) at low temperatures and after operational embrittlement, through extrinsic toughening by introducing crack energy dissipation mechanisms. Existing W_f/W samples produced via chemical vapor infiltration indeed showed higher toughness in mechanical tests than pure W. In this contribution W_f/W material specimens produced via powder metallurgical (PM) methods, e.g. hot isostatic pressing (HIP), are shown. A variety of measurements, e.g. 3-point bending and push-out tests, are presented to verify the operation of the expected toughening mechanisms. Therefore the focus of the investigations lies on the interface deboning behavior. In particular, the stability and integrity of the interface is investigated, since high temperatures (up to 1900 °C) and pressures (200 MPa) are present during the composite preparation. First HIP single-fiber samples indicate a compact matrix with densities of 99+ % of the theoretical density of W and showed signs of recrystallization and grain growth. SEM analysis demonstrates an intact interface with indentations of powder particles at the interface-matrix boundary. Push-out test results indicate that the structure of the interface may be damaged by HIPing since push-out of matrix elements is observed.

MM 28.30 Tue 18:30 Poster E

Effect of Mg addition on the mechanical properties of a Zn-Al-Cu alloy — •Zhicheng Wu, Liang Wu, Weiping Hu, Günter Gottstein, and Sandra Korte-Kerzel — Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-52074 Aachen, GERMANY

Zinc alloys are liable to creep even at only moderately elevated temperatures due to their low melting point of around 380°C. In order to increase the strength and especially the creep resistance of a Zn-Al-Cu alloy by solid solution and precipitation strengthening, the effect of Mg addition was studied. On the basis of the composition of the commercial alloy Z410 (4wt% Al, 0.5wt% Cu), three laboratory alloys were produced with different amounts of Mg (0.04wt%, 0.2wt% and 0.3wt%) and characterized in terms of their mechanical properties and microstructure using tensile tests in conjunction with scanning and transmission electron microscopy. Tensile tests were performed at RT, 55°C and 85°C and strain rates of 5×10^{-4}, 5×10^{-5} and $6\times10^{-6}/s^{-1}$. The true stress - true stain curves revealed at low strain rates (5×10^{-5} and $6\times10^{-6}/s^{-1}$) a regime with a nearly constant work softening rate. Based on the low strain rate tests, the steady state creep rate of the investigated Zn alloys was approximated in order to estimate the creep activation energy and stress exponent of the studied Zn alloys. It was found that the Zn alloy with medium Mg content (0.2wt%) had the highest yield strength both at RT and elevated temperatures and also the highest activation energy for creep. The underlying physical mechanisms of the observed phenomena will be briefly discussed.

MM 28.31 Tue 18:30 Poster E

Flow curve simulations of aluminum binary alloys — •Volker Pankoke[1], Volker Mohles[1], Philipp Schumacher[2], and Benjamin Milkereit[2] — [1]RWTH Aachen Univerity, Institute of Physical Metallurgy and Metal Physics, Aachen, Germany — [2]University of Rostock, Chair of Materials Science, Rostock, Germany

A work hardening model based on four different types of dislocation densities is used to calculate flow curves of aluminum alloys in a temperature range from 30 to 500°C and strain rates of 0.1 and $0.001s^{-1}$. Experimental input comes from stress strain curve measurements on Al-Si alloys with different Si content and precipitates, depending on

the cooling rate settings of the alloy. During cooling the precipitation behavior of the samples is investigated by Differential Scanning Calorimetry (DSC) to measure and control precipitation. To describe the plasticity of the alloys with the Four Internal Variable Model (4IVM), solute atoms must be taken into account. The corresponding formulation of the previous model 3IVM+ failed for the Al-Si alloys under consideration. Several approaches were tested in order to develop a new model for solid solution strengthening. Among them are the assumption of a short range order stress which depends on temperature but not on the different strain rates. Additionally the effect of Cottrell-clouds is implemented in the model, which leads to a range of abnormal thermal dependence of the flow stress and to jerky flow under certain conditions. The simulated flow curves and their serrations are compared to the measurements.

MM 28.32 Tue 18:30 Poster E

Strong correlation between acoustic and electromagnetic emissions during plastic deformation and destruction in solids — Dimitris Mastrogiannis[1], Tatiana Antsygina[2], •Konstantin Chishko[2], Claire Mavromatou[1], and Vassilios Hadjicontis[1] — [1]University of Athens, Panepistimiopolis, Zografos, TK 157 84, Athens, Greece — [2]B. Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., 61103 Kharkov, Ukraine

Simultaneous acoustic (AE) and electromagnetic (EME) emissions during uniaxial compression of LiF monocrystals and polycrystalline natural rocks are studied experimentally and interpreted theoretically. It is proved the strong correlation between AE and EME in solids of different types. It means that both AE and EME have the same physical background in evolution of crystal lattice defects (dislocations, vacancies, cracks) during plastic deformation and destruction, despite the different ways to form acoustic or electromagnetic response from the same deformation act. Generation of EME is due to macroscopic polarization currents generated by dynamic lattice defects. In ionic crystals the currents are produced through pinning-unpinning between charged vacancies and dislocation lines which can transport the vacancies on macroscopically long distances. Granites are piezoelectric composites where deformation is mainly due to microcracking acts. Electromagnetic signal in this case forms within two steps: first, a short pulse from free charge re-distribution at crack nucleation, and, second, an electromagnetic satellite of emitted acoustic wave. EME is prospective for practical applications in areas where the only AE was used before.

MM 28.33 Tue 18:30 Poster E

(Nano-)Mechanical properties of intermetallic phases in the Fe-Mo system at elevated temperatures — •Sebastian Schröders and Sandra Korte-Kerzel — Institut für Metallkunde und Metallphysik, RWTH Aachen University, Kopernikustrasse 14, 52056 Aachen, Deutschland

Topologically close packed (TCP) intermetallic phases which precipitate in nickel-base superalloys are suspected to cause a deterioration of the mechanical properties of the γ - γ* matrix. Although the existing intermetallics, namely Laves-, R-, sigma- and mue-phases are well understood in terms of their structure, their mechanical properties have still not been investigated in detail due to their size and pronounced brittleness. In order to investigate the plastic deformation behavior of these phases, but exclude the effect of complex phase composition in the first instance, the Fe-Mo system was chosen as a model system, where all phases are available as binary alloys. Using nanomechanical testing methods like nanoindentation and micropillar-compression, the experimental challenges of high brittleness and anisotropy encountered in conventional testing can be disregarded and plastic deformation can be achieved due to the confining pressure in nanoindentation and the reduction in specimen size in microcompression. This work aims to examine the mechanical properties such as elastic modulus, yield and flow stress of intermetallic Fe-Mo phases over a range of temperatures. To this end, tests were performed in vacuum. Based on this type of study it is envisaged to form a better understanding of the way hard TCP precipitates influence the performance of superalloys.

MM 28.34 Tue 18:30 Poster E

Influence of heterogeneities on the fracture behavior of NiAl — •Polina N. Baranova, Johannes J. Möller, and Erik Bitzek — Department of Material Sciences & Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

The fracture of a brittle solid is crucially determined by material heterogeneities directly at the crack front where the stress field diverges. Here, the usual homogenization strategies of continuum mechanics are no longer applicable, and currently there exist no consistent theory that relates local fluctuations in elastic properties, cohesion, toughness, or stress fields to the local fracture behavior and macroscopic failure criteria. Here we present atomistic simulations of static and propagating cracks in the Ni-Al system to study the influence of heterogeneities on the fracture behavior. Heterogeneities on the atomic scale were introduced by varying the composition of B2 NiAl, whereas voids and Ni-precipitates served as mesoscale heterogeneities. The simulation results are compared to experiments and discussed in the framework of linear elastic fracture mechanics for heterogeneous media.

MM 28.35 Tue 18:30 Poster E

Applying the concept of gradient elastic tensors in the determination of dislocation densities in MAX phases — Christoph Brüsewitz[1], Ulrich Vetter[1], •Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

MAX phases provide an unusual combination of both metallic and ceramic properties. Their remarkable mechanical properties, especially their damage tolerance, are still not fully understood and are subject of current debates. In this context, a way to *in-situ* determine dislocation densities under deformation would be most helpful.

We will present an attempt for this determination that is based on an hyperfine interaction method, the perturbed angular correlation spectroscopy, by using the sensitivity of the electric field gradient (EFG) at a nucleus on the strain field of defects. The relevant parameter is the broadening of the EFG tensor components. The coupling between EFG tensor and strain field is generally described by the gradient elastic tensor whose structure is determined by the point group of the corresponding nucleus. In case of the MAX phases, the tensor components are experimentally not determinable which is why density functional theory calculations implemented in Wien2k were used instead. Based on these calculations, a first estimation of deformation induced dislocation densities is given.

MM 29: Invited talk Dunlop

Time: Wednesday 9:30–10:00 Location: TC 006

Invited Talk MM 29.1 Wed 9:30 TC 006

The role of geometric boundaries on shape changes in biology — •John Dunlop — Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Biological materials, can change shape and volume allowing organisms to form new tissue during growth and morphogenesis, as well as to repair and remodel old tissues. In addition such changes can also lead to useful motion or force generation (actuation) that may even still function in the dead organism, as seen in the example of the pine cone. Both growth and actuation of tissues are mediated by the physical constraints of the surrounding environment and the architecture of the underlying tissue. We explore the role of these geometric constraints by combining theoretical approaches with physical models made using advanced 3D printing technology, that can be tested either in cell-culture or in mechanical testing. This presentation will give an overview of this approach, highlighted by one example on growth and another on actuation. We will first show that by controlling the shape of pores inside scaffolds for tissue engineering it is possible to control the rate of new tissue formation [1]. Secondly we demonstrate how the pore shape in swellable honeycombs, can control macroscopic actuation behaviour [2]. Finally we hope to give an insight in how physical ideas stemming from such studies can be used to design new materials for medicine and robotics. [1] Bidan, C. M., et al (2013). Adv Healthcare Mater, 2, 186*194. [2] Guiducci, L.,et al (2014). J Roy Soc Int 20140458.

MM 30: Methods in Computational Materials Modelling III: Thermodynamics

Time: Wednesday 10:15–11:45 Location: H 0106

MM 30.1 Wed 10:15 H 0106

Magnetic materials at high temperature from first-principles: disordered magnetism, vibrations, phase stability and magnetic exchange interactions — •Björn Alling — Department of Physics, Chemistry, and Biology, Linköping University, Sweden

First-principles based approaches faces considerable challenges in modeling magnetic materials at high temperature due to the complexity of simultaneously treat the relevant magnetic, vibrational, and structural excitations. Here a first-principles framework is presented capable of calculating thermodynamic and magnetic properties of magnetic materials in their high-temperature paramagnetic state.

Calculations of temperature dependent vibrational spectra, Gibbs free energies and corresponding phase stabilities are based on the disordered local moments-molecular dynamics (DLM-MD) [2,3] The phonon spectra and pressure-temperature dependent phase transition of the hard coating material CrN is derived [5].

Furthermore, the effects of vibrations and structural disorder on the magnetic exchange interactions are derived. We use our approach to calculate the magnetic interactions of amorphous CrN illustrating the effects on magnetism in an extreme case of structural disorder. [6]

[1] B. Alling, T. Marten, and I. A. Abrikosov, Nature Materials 9, 283 (2010) [2] P. Steneteg, B. Alling, and I. A. Abrikosov, PRB 85, 144404 (2012) [3] B. Alling, L. Hultberg, L. Hultman, and I. A. Abrikosov, APL 102, 031910 (2013) [5] N. Shulumba, B. Alling, et al., PRB 89, 174108, (2014) [6] A. Lindmaa, R. Lizaraga, E. Holmström, I. A. Abrikosov, and B. Alling, PRB 88, 054414 (2013)

MM 30.2 Wed 10:30 H 0106

Phonon modes in Binary Crystals with Positional Disorder — •Tadeus Ras and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Classical DFT relates equilibrium density fluctuations $\delta\rho(\mathbf{q})$ to elastic response [1]. We present the dispersion relations of binary crystals following an approach to crystal elasticity that includes positional disorder [2].

Even a simple Ramakrishnan-Youssouf DFT of binary hard sphere systems predicts a variety of crystalline phases such as disordered fcc [3]. We illustrate the computation of both acoustical and optical phonon eigenfrequencies $\omega(\mathbf{q})$ of these phases in the presence of point defects. Further we point out the link of $\omega(\mathbf{q})$ to mechanical instabilities that may lead to martensitic phase transitions.

$\omega(\mathbf{q})$ can also be derived from the fluctuations $\delta\rho(\mathbf{q})$ itself. We finally refer to a straighforward method of evaluating experimental or simulation positional data.

[1] M. Fuchs, 'Elastic properties of colloidal solids with disorder', Proceedings of the International School 'Enrico Fermi' (2013).
[2] C. Walz and M. Fuchs, Phys. Rev. B, **81** (2010) 134110.
[3] S. W. Rick and A. D. J. Haymet, J. Phys. Chem., **94** (1990) 5212.

MM 30.3 Wed 10:45 H 0106

Sampling of temperature-dependent interactions within the cluster-expansion framework — •Sascha B. Maisel, Albert Glensk, Dominique Korbmacher, Tilmann Hickel, Blazej Grabowksi, and Jörg Neugebauer — Max-Planck Institute for Iron Research, Max-Planck Strasse 1, 40239 Duesseldorf, Germany

Temperature-dependent effective interactions are an enormous improvement over classical n-body Hamiltonians for a variety of reasons. Advantages include a better description of an alloy's remnant solubility in the dilute limit and more accurate predictions at high temperatures, where phonons are non-neglibible. We compare two different methods for sampling such temperature-dependent interaction strengths for the cluster-expansion method. The first method extends upon earlier work by Reith *et al.*, by including quasi-harmonic and electronic excitations contributing to the Gibbs free energy based on density functional theory phonon calculations. The second method samples temperature-dependent effective interactions directly from finite temperature *ab-initio* molecular dynamics simulations. Variations of this sampling procedure can deal with large interatomic relaxations far better than conventional sampling. We discuss the advantages, shortcomings and computational cost of both methods based on preliminary results for the Ni-Ti and Al-Sc systems.

MM 30.4 Wed 11:00 H 0106

***Ab initio* description of unstable phases at finite temperatures: The Ti bcc to ω transition** — •Dominique Korbmacher, Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti-based alloys are a technologically important class of structural materials. A detailed knowledge of their phase diagrams and transitions is important for optimizing the properties of these alloys. However, the occurrence of phases that become thermodynamically and dynamically stable only at high temperatures makes an ab initio computation of phase diagrams a challenging task.

We have therefore developed and applied an *ab initio* based methodology that allows to accurately compute free energies even of unstable phases. The method employs thermodynamic integration starting from a reference of optimized embedded atom potentials that were fitted to reproduce *ab initio* molecular dynamics data for a narrow volume and temperature range. We apply our technique to the bcc phase of pure Ti and compute its free energy up to the melting point. Our results show a second order phase transformation at around 1000 K upon lowering the temperature. A careful investigation of the molecular dynamics trajectories allows us to identify the low temperature phase as the technologically important hexagonal ω structure.

MM 30.5 Wed 11:15 H 0106

First principles study of competing phases in binary Ti-Ta alloys — •tanmoy chakraborty, jutta rogal, and ralf drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Ti-Ta shows a stable reversible martensitic phase transformation with a transformation temperature well above 350 K. This makes the material relevant for high temperature shape memory alloy (HTSMA) applications. In our study we use density-functional theory (DFT) in combination with the solid-state nudged elastic band (SSNEB) method to analyse the minimum energy paths along the transformation between different phases. From the relative stability of the phases as a function of Ta concentration we estimate trends in transformation temperature. The calculated phonon spectra provide insight into the dynamical stability of the phases and are used to assess thermal properties. Our results predict a range of 20-35 at.% Ta to be most suitable for a stable Ti-Ta based HTSMA.

15 min. break

MM 31: Liquid and Amorphous Metals IV: Structure and Electronic Properties of Glasses

Time: Wednesday 10:15–11:30 Location: H 0107

MM 31.1 Wed 10:15 H 0107

Computer simulations of glasses: the potential energy landscape — •Zamaan Raza, Björn Alling, and Igor Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping 581 83 SWEDEN

Interest in amorphous materials and glasses is increasing with the advent of physical vapour deposition techniques that are capable of creating ultrastable metallic glasses with properties that can only otherwise be be achieved by aging a glass formed from a supercooled liquid by thousands of years. However, our understanding of the microscopic structure of glasses is poor, and our ability to model them using *ab initio* techniques is limited. We discuss the potential energy landscape paradigm to account for the phenomenology of structural glasses, and the way in which it can be applied in simulations and the interpretation of their results. Our aims include determining a parameter that describes glass-forming ability from first principles, and developing methods for generating high quality structural models of glasses and amorphous solids.

We consider amorphous boron carbide as an example. With a worldwide shortage of ^{3}He, an affordable neutron detecting material is required for projects such as the European Spallation Source (ESS). In spite of its unique properties, including a high neutron-capture cross section, self healing and high mechanical strength, its structure is still poorly understood; for example, it is unknown whether it has an intrinsic length scale.

MM 31.2 Wed 10:30 H 0107

On the process of structure formation and emergence of properties in AlMnCu — •Syed Sajid Ali Gillani, Steffen Schulze, and Peter Häussler — Chemnitz University of Technology, Physics Institute, 09107 Chemnitz

Most AlTM-alloys (TM : transition metal), which become amorphous for less than 60 at%TM, whereas AlMn stays amorphous up to much higher Mn-contents. The different influence of Mn may depend on its unique properties compared to the other 3*d*-TMs. It has outstanding structural and magnetic properties and hence is claimed to be one of the most complex elements. In its pure state it has three different crystalline phases which causes strong disorder, seen e.g. by its very high resistivity, as high as the surrounding elements in the Periodic Table have in their liquid state. To get a deeper insight we replace partially Mn by Cu along two different cuts through the corresponding ternary AlMnCu. Here we report on the emerging structural and physical transport properties and discuss the particular role of the TM.

Our analysis is based on self-organizing global *spherical-periodic* resonance effects between the Fermi gas and the forming static structure. The global resonances are self-organizing by their exchange of characteristic momenta. They trigger particle-density anomalies, hybridization effects as well as phase separation. The corresponding structure factors $S(K)$ shows the resonance peak at $K_{\mathrm{pe}}=2k_{\mathrm{F}}$, indicating a *spherical-periodic* atomic order in r-space. The self-organizing processes are limited since e.g. hybridization needs minimal as well as maximal contents of TMs and depends on the chosen TM.

MM 31.3 Wed 10:45 H 0107

Structure and electronic properties of amorphous In-Mn-alloys — •Benny Böhm, Syed Sajid Ali Gillani, Martin Stiehler, Steffen Schulze, and Peter Häussler — Technische Universität Chemnitz, D-09107 Chemnitz

Basic principles during structure formation have been reported in former contributions for binary amorphous Al-transition metal-alloys (*a*-Al-TM). Presently, Al in those alloys has been replaced by other elements of the boron group and the focus hence has shifted to *a*-Ga-Mn and *a*-In-Mn. Here we report on the latter. Structure and properties emerge from the coupling of two global subsystems, the Fermi gas and the structure-forming ions. Along several degrees of freedom and via an exchange of momentum they come into resonance and form a new equilibrium. Under resonance the electronic dispersion forms a pseudogap at E_{F} with consequences on structure, its thermal stability, and electronic transport.

Thin films of In-Mn with different compositions from 40 - 70 at%Mn were deposited at low-T. The electrical resistivity up to several hundred Kelvin was measured and electron diffraction performed on a TEM at T=350 K. Close to this temperature *a*-In-Mn-alloys, unfortunately, seem to segregate into two phases, shows two main structural peaks in its structure factor S(K). One seems to be related to pure In, the other one to a phase which is still amorphous at T=350 K. Due to the two peaks in real space structural beats in the pair-distribution function g(r) occur. Transport properties support these indications.

MM 31.4 Wed 11:00 H 0107

Structure and electronic transport of amorphous Ga-Mn alloys — •Leopold Koch[1], Hans Weber[2], Martin Stiehler[1], Steffen Schulze[1], and Peter Häussler[1] — [1]Technische Universität Chemnitz, 09107 Chemnitz — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Helmholtzstraße 20, 01069 Dresden

The last years we reported on structure formation in binary amorphous Al-transition metal alloys (*a*-Al-TM). The formation of structure is the result of global resonance effects between the Fermi gas and the forming static structure. The resonance causes a pseudogap at $\mathrm{E_F}$ and defines the observed transport properties. During structure formation the resonance gets optimized by hybridization effects between the TM-d- and Al-p-bands at E_{F}. While this behavior proved to be nearly independent on the particular TMs, the necessity of Al as the second element was unclear. Accordingly, Al has been replaced by other elements from the boron group, e.g. Ga or In. In the present contribution we report on structural and electronic properties of a-Ga-Mn alloys.

Thin films ($d \approx 50$ nm) were deposited in high-vacuum at low T. The electrical resistivity was measured during annealing to several hundred K, the static atomic structure at around 300 K. Pure Ga itself becomes amorphous at very low T, but crystallizes already around T=14 K. By adding Mn the stability rises tremendously and amorphicity could be achieved in a wide concentration range. The overall structural as well as the electric transport properties of a-Ga-Mn are very close to a-Al-Mn. The magnetic behavior still has to be measured.

MM 31.5 Wed 11:15 H 0107

Structure and electronic properties of Al-Pd-Alloys — •Pierre Pudwell, Martin Stiehler, Steffen Schulze, and Peter Häussler — Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz

During the last years we reported on the influence of resonance-like effects during structure formation in condensed matter physics. These are based on an internal exchange of momentum between global subsystems, namely the valence electrons and the forming static structure. Hereby both subsystems are able to adjust their internal properties along different degrees of freedom. Amorphous (a) alloys proved to be perfectly suited to explore the evolution of this mutual adjustment in detail. Structure formation, phase stability and electronic transport properties were found to be strongly related. Especially in a-Al-transition metal (TM) alloys, due to the TM-d-states at E_{F}, a high flexibility of the electronic subsystem was observed.

In the present contribution we report on binary a-Al-Pd alloys in the form of thin films (≈ 50 nm). For different concentrations in the range from 20 to 75 at.% Pd, we measured the resistivity from 4K to several hundred K. The static atomic structure and the plasma resonance were obtained after annealing to 350K in a transmission electron microscope, the latter using electron energy loss spectroscopy (EELS). Although the overall behaviour of Al-Pd is comparable with other Al-TM systems distinctive deviations become obvious.

MM 32: Biomaterials and Biological materials I

Time: Wednesday 10:15–11:45 Location: TC 006

Topical Talk MM 32.1 Wed 10:15 TC 006

Structure-property relations in biological composite materials: An inspiration source for synthetic materials — •Helge-Otto Fabritius[1], Joachim Enax[2], Xia Wu[3], Matthias Epple[2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]University of Duisburg-Essen, Essen, Germany — [3]University of Paderborn, Paderborn, Germany

From a materials science point of view, biological materials are hierarchically structured nano-composites optimized through evolution to perform vital functions within the specific eco-physiological strains of living organisms. Most of them consist of a matrix of structural biopolymers like collagen in vertebrate bones and teeth, chitin in arthropod exoskeletons, or cellulose in plants and various other organic and inorganic constituents. Their physical properties are adapted to the specific functions of the materials and can be very diverse, which is caused by structural and chemical alterations at different hierarchical levels. Understanding the structure-property relations and thus the design principles of biological materials is a valuable source of inspiration for the development and improvement of synthetic materials with tailored properties. Using a combination of experimental and theoretical approaches, we explore this potential in a variety of natural materials like shark tooth enameloid as a biological model for dental materials with improved performance and durability and photonic crystals formed by the arthropod cuticle as inspiration for the development of new, optically active materials.

Topical Talk MM 32.2 Wed 10:45 TC 006

Towards bioinspired adaptive composites using responsive microcapsules — •André R. Studart — Complex Materials, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Biological materials exhibit dynamic self-healing and adaptive functionalities that arise from the coordinated action of living cells. Despite the unparalleled complexity of biological systems, major efforts have been made to generate engineered microcompartments that partly replicate just a few key features of the fascinating dynamic response of living cells. In this talk, I will present our recent efforts to create chemically- and mechanically-responsive microcompartments using templating double emulsions made by a microfluidic technique. In the first part of the talk, I will present tools to obtain polymer-based capsules with predictable size and shell thickness, as well as tunable mechanical behavior and shell microstructure. Such microcapsules are incorporated into polymer matrices to generate composites with self-healing and adaptive properties. In the second part, I will describe a general strategy to create multifunctional colloidosomes that can release cargo on-demand in response to an external chemical trigger. This is achieved by reversibly trapping cargo molecules inside the colloidosome or by implementing gating properties to the capsule wall using responsive polymer shells. While the capsules obtained remain very far from reaching the responsiveness of truly dynamic biological systems, the level of geometrical and materials control enabled by microfluidics makes it a promising platform for the creation of advanced microcompartments for future capsule-based adaptive materials.

MM 32.3 Wed 11:15 TC 006

Banksia - fire-triggered seed release — •Michaela Eder[1], Vanessa Schoeppler[1], Jessica Huss[1], David Merritt[2], and Peter Fratzl[1] — [1]MPI for Colloids and Interfaces, Potsdam, Germany — [2]Botanical Gardens and Park Authorities, Perth, Western Australia

After germination plants are bound to a certain location which requires functionality of the material forming the plant body. Fascinating examples can be found in extreme environments such as fire-prone areas: the woody follicles of the Australian genus Banksia encapsulate and store seeds in the plant canopy, in some cases for more than 15 years, until they are released during/after fire. This requires both long-term (dimensional) stability and the ability for seed release triggered by fire. The two valves of the follicles are connected by a zone of interdigitating cells sealed with a wax/resin. Heat causes initial opening along this zone, but opening does not seem to be controlled by the melting temperature of the wax/resin. Instead the complex micro- and ultrastructure appears to control a 2-stage opening process. After initial opening by fire, wetting and drying cycles are required for seed release. This presumably ensures optimal conditions for germination are present (ie water availability) before seed release. From a biomimetic point of view detailed knowledge about material properties of the follicles can be useful for eg the development of environmental friendly, biomimetic flame retardants, the design of dimensional stable bio-based construction materials or the development of robust fire-sensors which may function as actuators.

15 min. break

MM 33: Structural Materials I: Phase Stability and Mechanical Properties

Time: Wednesday 10:15–11:30 Location: TC 010

MM 33.1 Wed 10:15 TC 010

Comparison of Co-X and Ni-X systems with density functional theory and bond-order potentials — •Jörg Kossmann, Alvin Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Single crystal superalloys are used widely in high-temperature applications. Most of todays superalloys are based on Ni-Al and comprise 10 or more alloying elements. For example, Re and other 5d elements are added to improve creep resistance. Recently, materials based on Co-Al-W where shown to possess a γ/γ' microstrcuture which makes these alloys interesting for singe crystal superalloy applications. We compare and contrast Co-based and Ni-based alloys from high-throughput density-functional theory (DFT) calculations. We relate phase stabilities, lattice constants, and elastic constants in Co-X and Ni-X binaries with X=Al,W,Re and the ternary systems Co-Al-W and Ni-Al-Re. New bond-order potentials (BOPs) are fitted to the DFT results and we obtain satisfactory agreement between BOP and DFT.

MM 33.2 Wed 10:30 TC 010

Analysis of the thermodynamic phase stability in the Al-Sc system using first principles methods — •Ankit Gupta[1], Biswanath Dutta[1], Tilmann Hickel[1], Jörg Neugebauer[1], Yulia Buranova[2], and Sergiy Divinski[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Institute of Materials Physics, University of Münster, D-48149 Münster, Germany

Driven by the need to achieve high strength materials with reduced weight, Al-Sc alloys have received considerable attention in the last couple of decades owing to their superior mechanical and anti-recrystallization behaviour. These improved properties critically depend on Al_3Sc particles that precipitate out from Sc supersaturated solid solution. In experiment, their shape, distribution and morphology show a remarkable variation depending on composition and mechanical load, which has not yet been understood. In this work, we therefore investigate the thermodynamic phase stability of this alloy system within a first-principles based approach with a focus on the Al rich corner of the binary phase diagram. The temperature dependence of the Sc solubility in Al is calculated as an outcome of a competition between the free energies of formation of the dilute solvents and the ordered precipitate phase within the quasi-harmonic approximation. Our results for the thermodynamic and elastic properties of the Al_3Sc phase additionally confirm the experimental finding of coherent precipitates. The investigations are extended towards kinetic Monte-Carlo simulations of the precipitation kinetics in terms of TTT diagrams for the precipitate formation.

MM 33.3 Wed 10:45 TC 010

Correlation between thermodynamic and mechanical properties in Ta-W — •Sandra Hoppe and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Varying an alloy's concentration or alloying constituents strongly influences its structural and mechanical properties. Modern simulation methods like density functional theory in combination with the cluster expansion make the whole configurational space accessible. This way, also metastable structures may be considered, which are experimentally difficult to obtain. 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 binary body-centered cubic (bcc) alloys. As a model system, Ta-W was chosen due to its simple phase diagram with solid solution in the whole concentration range. Interestingly, the elastic constants c_{44} and c_{12} show an opposing trend to that observed for fcc alloys: Energetically favorable structures are mechanically weaker than those further away from the ground-state line. This phenomenon may be related to the anomalous behavior of c_{44} with increasing pressure or temperature, which has been reported in the literature for Ta-W. We will discuss the interesting behavior of Ta-W with regard to its electronic structure.

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

MM 33.4 Wed 11:00 TC 010

From generalized stacking fault energies to dislocation cores: impact of solutes on the Peierls stress in magnesium — •Zongrui Pei[1,2], Martin Friák[3,1,2], and Jörg Neugebauer[1] — [1]1Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Aachen, Germany — [3]Institute of Physics of Materials of the Academy of Sciences of the Czech Republic, v.v.i, Brno, Czech Republic

Using ab initio calculations and Fourier transform we analyze a basal plane gamma surface in pure Mg and show that the knowledge of energies of only three specific points is sufficient to accurately predict the core structure of <a> dislocations. This finding greatly reduces the computational costs related to the Peierls-Nabarro (PN) model and allows for a high-throughput application of the PN model to dislocation cores in Mg alloys. We employ our approach to study Mg binary alloys containing 9 rare-earth (RE) and 11 other solutes that crystallize in either hexagonal close-packed (hcp) or double hcp (dhcp) structures. Based on the calculated core structures of these 20 Mg alloys, solutes are divided into three groups. The group consisting of Co, Os, Re, Ru, Tc and Ti shows more compact core structures and larger Peierls stress than pure Mg, the group including Be, Hf, Tl, Zn, Zr and Sc (the only RE element in this group) changes both the core widths and Peierls stresses moderately. The third group containing the other RE elements extend the core width from 9b-19b, and the Peierls stresses are generally very low, which shows a solute solution softening trend.

15 min. breack

MM 34: Structural Materials II: Brazing and Welding

Time: Wednesday 11:30–12:15 Location: TC 010

MM 34.1 Wed 11:30 TC 010

Eigenschaftsdegradation durch H in schweißgeeigneten höherfesten Feinkornbaustählen unterschiedlicher Herstellungsverfahren — •Enrico Steppan, Arne Kromm und Thomas Kannengiesser — Bundesanstalt für Materialforschung und -prüfung

Der Einsatz schweißge. höherfester FKB ist aus wirtschaftlichen Gründen & dem Streben nach konstruktivem Leichtbau in vielen Industriezweigen unabdingbar. Das Potential einer Sensibilität gegenüber H-bedingter Eigenschaftsdeg. ist jedoch signifikant erhöht. Die mech.-technolog. Gütewerte moderner niedriglegierter höherfester FKB werden maßgeblich durch Ihre chem. Zus. und dem Herstellungsprozess beeinflusst. Hierdurch leiten sich mikrostrukturelle Unterschiede (Korngröße, Ausscheidungen, Versetzungen) ab. Aufgrund dessen wurden 2 höherf. FKB gleicher Festigkeitsklasse, jedoch unterschiedlicher Herstellung (vergütet Q/thermomechanisch MC), untersucht. Neben den makroskopisch beobachtbaren Merkmalen (Streckgrenzenerhöhung, Abnahme wahre Bruchdehnung und Bruchfläche) wurde das lokale Verhalten unter H in den Stählen mit Synchrotronstrahlung am HZB untersucht. Anhand H-beladener Zugproben wurde die Wechselwirkung des H mit dem Gitter untersucht. Hierzu wurden entsprechende Messungen während des Zugversuches im elast., elast./plast. und plast. Bereich vorgenommen. Grundlegende Unterschiede zwischen den verwendeten Stahlgüten bezüglich der H-degradation ließen sich somit anhand makroskopischer als auch mikroskopischer Merkmale erstmals belegen. Die erlaubt schließlich Rückschlüsse auf die grundlegenden Mechanismen der Eigenschaftsdeg. durch H.

MM 34.2 Wed 11:45 TC 010

Analysis of interface layers in dissimilar Al-Ti FSW-Joints — •Roland Marstatt[1], Markus Krutzlinger[2], Johannes Luderschmid[1], Robert Bartel[1], Michael F. Zäh[2], and Ferdinand Haider[1] — [1]Lehrstuhl fuer Experimentalphysik I, Universitaet Augsburg, Augsburg, Germany — [2]Institut fuer Werkzeugmaschinen und Betriebswissenschaften (iwb), Technische Universitaet Muenchen, Garching, Germany

Friction Stir Welding (FSW) is a suitable technology to join dissimilar materials. In contrast to fusion welding processes the material does not exceed the solidus temperature during FSW. As a consequence FSW seems to be a good choice to form dissimilar joints as e.g. between aluminium and titanium alloys. Process optimization aims on the production of high quality dissimilar joints with a minimum of deleterious brittle 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 results of the formation of nano-scaled intermetallic layers at the bonding interface are presented. Therefore dissimilar joints of aluminium and titanium alloys, with lap as well as butt joint setups stirred only in aluminium, have been investigated under varying process conditions. The intermetallic layer plays a key role as joining mechanism - its thickness depends on process parameters and controls the static and dynamic mechanical properties of the joint. Understanding the relevant process parameters for the formation of this interlayer allows to control the joint quality.

MM 34.3 Wed 12:00 TC 010

Diffusion brazing of γ-TiAl-alloys: Investigations by high-energy XRD and electron microscopy — •Katja Hauschildt, Andreas Stark, Peter Staron, Helmut Eckerlebe, Uwe Lorenz, Norbert Schell, Florian Pyczak, and Martin Müller — Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Germany

Diffusion brazing is a promising method to close cracks (in noncritical or non-highly loaded areas) in parts made of TiAl alloy, 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 by high-energy X-ray diffraction (HEXRD) using the materials science beamline HEMS at the PETRA III synchrotron facility at DESY in Hamburg, Germany. In addition, first in-situ studies of the brazing process were performed. Furthermore, the microstructure was characterised by scanning electron microscopy (SEM) including energy-dispersive X-ray spectroscopy (EDX) and electron backscattered diffraction (EBSD). Additionally, tensile tests at room temperature were carried out. The combined results show, that the brazing zone is composed of two or three transitional layers from substrate material to the middle of the joint. While the phase constitution close to the substrate material resembles a TiAl-alloy, the microstructure in the middle of the joint is similar to α/β-titanium alloys.

MM 35: Methods in Computational Materials Modelling IV: Steels

Time: Wednesday 11:45–13:15 Location: H 0106

MM 35.1 Wed 11:45 H 0106

Temperature-dependent magnon-phonon coupling in bcc Fe — •Fritz Körmann, Blazej Grabowski, Biswanath Dutta, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

An ab initio based framework for quantitatively assessing the non-adiabatic free energy contributions due to magnon-phonon interactions and lattice expansion to phonon energies is developed [1]. Employing the framework of the recently developed spin-space averaging (SSA) procedure provides paramagnetic forces at high temperatures [2]. The full temperature dependence of phonons for arbitrary magnetic temperatures is obtained by relating the ferromagnetic and paramagnetic SSA force constants with energetics from the magnetic subsystem. The latter is derived by means of QMC simulations for an effective Heisenberg model [3]. The theoretical results for bcc Fe are in very good agreement with recent high-quality phonon frequency measurements [1]. For some phonon branches, the impact of magnetic excitations is an order of magnitude larger than the phonon shift due to lattice expansion. The significant role of magnetic short-range order on lattice vibrations above the Curie temperature is demonstrated.

[1] F. Körmann, B. Grabowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, J. Neugebauer, Phys. Rev. Lett. 113, 165503 (2014).

[2] F. Körmann, A. Dick, B. Grabowski, T. Hickel, J. Neugebauer, Phys. Rev. B 85, 125104 (2012).

[3] F. Körmann, A. Dick, T. Hickel, and J. Neugebauer, Phys. Rev. B 83, 165114 (2011).

MM 35.2 Wed 12:00 H 0106

Characterisation of transformations at disordered FeCr bcc-σ interfaces — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Using an adaptive kinetic Monte Carlo (akMC) approach, we study the transformation of the σ-phase in FeCr to the bcc structure. During the transformation we observe disordered interface regions with a thickness of several atomic layers. Transformation paths from one crystal phase to another become obfuscated by seemingly random movements and rearrangements at the interface. This creates a challenge in studying the atomistic processes that drive the transformation.Based on our akMC trajectories we analyse the topology of the potential energy surface and the influence of excessive loops on the transformation paths. Using coordination polyhedra and topological fingerprints we look for correlations in processes in the interface region of FeCr bcc-σ interfaces and along the transformation paths trying to identify characteristic processes of the phase transition.

MM 35.3 Wed 12:15 H 0106

Multi-scale description of super-saturated ferrite in severely deformed pearlitic wires — •Nematollahi Gh. Ali, Grabowski Blazej, Raabe Dierk, and Neugebauer Jörg — Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany

Severely deformed pearlitic wires are the strongest structural materials with up to 7 GPa strength. Despite extensive research the fundamental mechanisms underlying the extraordinary strength are unclear. Experimental evidence suggests a substantial cementite decomposition resulting in a dramatically increased C concentration in the ferrite matrix which is 9 orders of magnitude above phase diagram predictions. To study the stability of C interstitials in ferrite and of C vacancies in cementite in the presence of elastic strain and dislocations we have developed a multi-scale approach using density functional theory, embedded atom potentials and an empirical model. A careful analysis reveals that a strain-induced stabilization of the C interstitial in ferrite in conjunction with a stabilization of the C trapping sides around dislocations enhance the carbon solubility strongly. Based on this insight we are able to explain the experimentally observed super-saturation of ferrite and the partial dissolution of cementite in severely deformed pearlite.

MM 35.4 Wed 12:30 H 0106

Z phase strengthened steels for ultra-supercritical power plants — •Daniel F. Urban, Christian Elsässer, and Hermann Riedel — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

To minimize fuel consumption and CO2 emission of fossil fired power plants, the thermal efficiency, and therefore the steam inlet temperatures, must be as high as possible. In the past 30 years sufficiently creep resistant 9% chromium steels were developed, allowing steam temperatures up to 615 °C. The increased creep resistance was obtained by controlled precipitation of fine (V,Nb)N particles. Further raise of the steam temperature calls for higher Cr contents for better corrosion and oxidation resistance. However, 11-12% Cr ferritic-martensitic steels strengthened by fine (V,Nb)N particles reveal that precipitation of the thermodynamically stable Z-phase, Cr(V,Nb,Ta)N, in long-term service is unavoidable and detrimental. Usually, coarse and brittle Z-phase particles grow at the expense of the desired fine nitride particles. We follow the idea to exploit the Z-phase as strengthening agent in martensitic creep resistant 12% Cr steels by controlling the precipitation of the Z-phase such that fine, thermodynamically stable Z particles are formed. We present atomistic DFT simulations which reveal the essential mechanisms underlying the Z-phase formation. Chromium atoms diffuse into nitride particles and subsequently cluster in a layered arrangement which finally yields the transformation of the nitride particles to Z-phase.

MM 35.5 Wed 12:45 H 0106

Calculation of Electronic Thermophysical Parameters for Steel Alloys based on Density Functional Theory — •Juergen Sotrop[1], Jan Winter[1], Heinz P. Huber[1], Stephan Borek[2], and Jan Minar[2,3] — [1]Munich University of Applied Sciences — [2]Ludwig-Maximilians Universit, Muenchen — [3]University of West Bohemia, Pilsen

The ablation mechanism of matter irradiated with ultra-short laser pulses has been widely investigated over the last two decades. At present there is still lack of theoretical understanding of the interaction of ultra-short laser pulses with a metal alloy. By irradiating material with ultra-short laser pulses initially strong electron-phonon nonequilibrium will occur. The resulting difference in electron and phonon temperatures can be calculated with the so called two-temperature model (TTM). An essential prerequisite for the application of the TTM is a determination of the temperature dependent thermophysical parameters such as electron heat capacity and electron-phonon coupling factor. We will present a general method for the calculation of the electronic thermophysical parameters for metal alloys, here performed exemplarily on stainless steel (AISI 304). The method is based on the calculation of the electronic density of states (DOS) using a fully relativistic implementation of the KKR-formalism in the framework of spin density functional theory. Precise knowledge of the DOS will enable the calculation of the electron-phonon-coupling factor and the electron heat capacity. The model is compared with the well-known parameters for iron to show the validity.

MM 35.6 Wed 13:00 H 0106

New metastable phases of the Cr_xSb_y system with different $x:y$ ratios: theory and experiment — •Svitlana Polesya[1], Gerhard Kuhn[1], Sergiy Mankovsky[1], Matthias Regus[2], Wolfgang Bensch[2], and Hubert Ebert[1] — [1]Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Str. 2, D-24118 Kiel, Deutschland

The present investigation aims to find new metastable phases of the Cr-Sb system as well as of some other compounds based on it. Corresponding experimental investigations are supported by theoretical first principle calculations which allow to predict the physical properties of new compounds and alloys and to explain the behaviour of new phases synthesized experimentally. In particular we focus on the Cr_xSb_y compounds with the ratios $x:y = 2:1, 1:2$, and $1:3$. In the case of the non-stoichiometric $Cr_{1+x}Sb$ compound a new Cr-rich phase has been obtained which crystallizes in the Ni_2In-like structure. The structure parameters for this system obtained via ab-initio total energy calculations are in good agreement with the experimental values. The calculations demonstrate the preferential layer-like occupation by Cr of the interstitial sites in the compound and clearly show its metallic behaviour. In the case of the Cr_xSb_y system with the ratios $x:y = 1:2$ and $x:y = 1:3$, the calculations have been performed for different possible structures, demonstrating their physical properties expected to be observed experimentally.

MM 36: Nanomaterials I: Excess Volume and Confinement

Time: Wednesday 11:45–12:45 Location: H 0107

MM 36.1 Wed 11:45 H 0107

Redistribution of Excess Volume by Mechanical Deformation in Nanocrystalline Alloys — •Michael Johannes Deckarm, Timo Tscharntke, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, D-66123 Saarbrücken

Nanocrystalline (NC) alloys with grain sizes at the low end of the nanoscale (≈ 10nm) are characterised by a large volume fraction of grain boundaries (> 25%), contributing to dramatically increased total excess volume and energy compared to conventional materials. We try to shed light on the interplay between these excess quantities and the altered mechanical properties of NC metals. Using a combination of X-ray diffraction, length and density measurements to detect direction-dependend and absolute excess volume changes before and after uniaxial compression, enabled us to compare our findings qualitatively with the predictions made by Bachurin and Gumbsch in (1). They simulated (MD-simulation) uniaxial deformedation of NC Pd and deduced an anisotropic redistribution of the grain boundary excess volume and an anisotropic change of Young's modulus. In contrast, we found no evidence for excess volume redistribution but rather an excess volume annihilation along the direction of compression. A possible reconciliation might be related to viscoelastic recovery processes.

(1) D. V. Bachurin, P. Gumbsch, Physical Review B, 85, (2012), 085407 1-9, doi:10.1103/PhysRevB.85.085407

MM 36.2 Wed 12:00 H 0107

Defects and structural anisotropy of HPT- and ECAP-deformed Ni studied by difference dilatometry — •Jaromir Kotzurek[1], Anton Hohenwarter[2], Simon Trubel[3], Christian Neubauer[1], Sergiy Divinski[3], Wolfgang Sprengel[1], Gerhard Wilde[3], Reinhard Pippan[4], and Roland Würschum[1] — [1]Institute of Materials Physics, Graz University of Technology — [2]Department of Materials Physics, University of Leoben — [3]Institute of Materials Physics, University of Münster — [4]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences Leoben

Difference dilatometry is used to study the excess volume associated with defects which are induced by high-pressure torsion (HPT) and equal-channel angular pressing (ECAP). Based on our recent studies of grain-boundary excess free volume in HPT-deformed Ni [1], issues of structural anisotropy and method of deformation are in the focus of the present studies. Both HPT- and ECAP-deformed nickel show an anisotropic defect annealing behavior prior to the onset of recrystallization, which can be associated with an anisotropic grain shape caused by the deformation. Anisotropic length change is also found after uniaxial post-deformation of HPT-Ni, indicating that the anisotropy is not caused by residual stresses. Financial support by the FWF Austrian Science Fund is appreciated (project P25628-N20).

[1] E.-M. Steyskal et al, Phys.Rev.Lett., **108** (2012) 055504

MM 36.3 Wed 12:15 H 0107

Charakterisierung der Nanoporen in mit Ionic Liquid beladenem Silica Gel über die Messung der Positronenlebensdauer — •Christian Herold — Technische Universität München, München, Deutschland

In diesem Beitrag werden Messungen an unterschiedlichen Silica Gel Proben vorgestellt, die mit einem Ionic Liquid (IL) beladen sind. Supported Ionic Liquid Phase (SILP) Materialien besitzen großes Potential für Anwendungen sowohl in Wissenschaft als auch in Industrie, u.a. als Katalysatoren. Mittels Positronen-Annihilations-Lebensdauer-Spektroskopie (PALS) war es uns möglich, das mittlere Volumen der Nanoporen im Silica Gel zu bestimmen. Dieses freie Volumen wird durch die Beladung mit IL und/oder Wasser drastisch reduziert. Bei einer Beladung mit 70 Volumenprozent IL ist das mittlere Porenvolumen gegenüber reinem Silica Gel um ca. 60% verringert.

MM 36.4 Wed 12:30 H 0107

Local sublattice symmetry breaking in graphene with centro-symmetric deformations — Martin Schneider[1], Daiara Faria[2], •Silvia Viola Kusminskiy[1], and Nancy Sandler[3] — [1]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universitaet Berlin, Deutschland — [2]Universidade Federal Fluminense, Rio de Janeiro, Brasil — [3]Ohio University, Ohio, United States

A generic deformation of a graphene sheet causes inhomogeneous strain which results in an effective, non-uniform pseudomagnetic field acting on the Dirac fermions. This can provide an alternative route to confine and control charge carriers in graphene. We investigate the electronic properties of a graphene sheet in the presence of an out-of-plane deformation with centro-symmetric geometry, for which the pseudomagnetic field presents trigonal symmetry. We address the question of confinement of electrons due to this deformation, using a scattering formalism based on the continuum description of graphene. In particular we study the local density of states (LDOS) of the electronic carriers, and show that this type of deformation causes a noticeable imbalance in the distribution of charge density between the two graphene inequivalent sublattices even for small deformations. We perform exact numerical calculations and show that the results are well described within an analytical, perturbative approach for small deformations. We discuss our results in view of recent experimental findings.

MM 37: Biomaterials and Biological Materials II

Time: Wednesday 11:45–13:15 Location: TC 006

MM 37.1 Wed 11:45 TC 006

Smart wooden actuators — •Markus Rüggeberg[1,2], Mohammad M. Hassani[1], Chiara Vailati[1,2], Falk Wittel[1], Hans J. Herrmann[1], and Ingo Burgert[1,2] — [1]ETH Zürich, Institute for Building Materials, Zürich, Switzerland — [2]Empa, Applied Wood Materials, Dübendorf, Switzerland

Wood swells and shrinks when exposed to fluctuating relative humidity. This property is a drawback for the use of wood as construction material. On the other hand the dimensional instability is the basis for creating smart, autonomously controlled actuators. Nature has developed numerous actuators responding to alternating relative humidity. In pine cones, wheat awns and orchid tree seedpods, the dimensional changes are transformed to bending and twisting movements by creating bi-layered structures with specific fibre orientations in the individual layers. Inspired by these plant model systems, we have developed convertible wooden elements. In outdoor applications, these elements respond to the daily alteration of relative humidity. Therefore, the movement of these elements is autonomous and solar driven. We compare experiments with numerical predictions using a rheological model of wood. A history dependent moisture-stress analysis using the developed material model under changing climatic condition is performed, to predict the true stress and deformation state. Possible applications are facades, or carriers of solar panels which autonomously track the sun. Upscaling of the actuators have already been demonstrated and a prototype of a carrier for solar panels has been successfully tested.

MM 37.2 Wed 12:00 TC 006

Moisture driven actuation of silica structures replicated from pine cone scales — •Gerhard Fritz-Popovski[1], Daniel Van Opdenbosch[2], Roland Morak[1], Oskar Paris[1], and Cordt Zollfrank[2] — [1]Institute of Physics, Montanuniversitaet Leoben Franz-Josef-Str. 18, 8700 Leoben, Austria — [2]Fachgebiet Biogene Polymere, Technische Universität München am Wissenschaftszentrum Straubing Schulgasse 16, D-94315 Straubing, Germany

The actuation behavior of silica structures that were based on the templates of pine cones was investigated. The silica structure replicated all structures from the macroscopic level down to the level of microfibrils (diameter 10-20 nm). While the movement of native pine cones is based of different swelling of the fibrous materials in fiber direction and normal to it the biotemplated silica material contains no fibers

but pores. Nevertheless, the inorganic material shows similar moisture dependent movements as the biological one. This can be explained by different elastic deformation of the pores along and normal to the axis during vapor condensation.

MM 37.3 Wed 12:15 TC 006

Self-folding polymer films for cell encapsulation and release — •Vladislav Stroganov and Leonid Ionov — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Deutschland

Asymmetry is intrinsic to natural systems and is widely used by living organisms for efficient adaptation, mimicry and movement. Polymer bilayers are the example of synthetic asymmetric systems, which are able to generate macroscopic motion and fold by forming different 3D objects such as tubes and capsules. Similar to bimetal films, the polymer bilayer consist of two substances with different swelling properties. One polymer is non-swellable and hydrophobic. Another polymer is water-swellable hydrogel. The folding, which might occur in response to temperature or pH, is caused by swelling of the hydrogel layer. The formed tubes and capsules can be manipulated using magnetic field. Reversible folding and unfolding of the polymer films is applied for reversible capture and release of cells in response to change of temperature and other signals. This novel biomimetic approach can be used for controlled encapsulation and release of microparticles, cells and drugs as well as fabrication of 3D scaffolds for tissue engineering.

Topical Talk MM 37.4 Wed 12:30 TC 006

Architectured strength: when tasty nuts and teeth meet: — •Claudia Fleck[1], Paul Zaslansky[2], Wolf-Dieter Müller[3], Andreas Bührig-Polaczek[4], and Thomas Speck[5] — [1]Materials Engineering, Institute of Technology, Berlin, Germany — [2]Julius-Wolff-Institute, Charité, Berlin, Germany — [3]Biomaterials Research and Dental Materials Science, Charité, Berlin, Germany — [4]Foundry Institute, RWTH, Aachen, Germany — [5]Plant Biomechanics, University Freiburg, Freiburg, Germany

In nature, damage tolerant tissues or organs ensure survival, by failing safely. Failure of the whole structure is delayed to allow repair processes, or it is even stopped, leaving behind a locally damaged, but still functioning entity. Many damage tolerant structures exist, even without self-healing capacity, and often the border between material and architecture is blurred. Mammalian teeth and Macadamia nutshells are two impressive examples. Chewing loads on whole teeth are distributed and transferred into the jaw bone by an intricate architecture of hard and soft materials, preventing failure even over millions of loading cycles. Macadamia nutshells protect the seed, despite numerous inner notches, by a multi-level sandwich and foam structure paired with a ball-like macro-geometry. We apply mechanical testing, in situ with light/electron microscopy or lab/synchrotron microtomogrpahy, together with FE-calculations, to characterize the structural reasons of failure resistance, and we aim at developing architectured metal or ceramic constructs with enhanced damage tolerance as compared to the monolithic materials.

MM 37.5 Wed 13:00 TC 006

Mapping internal mineral strains in human dentine under tension: X-ray diffraction insights into the contribution of the mineral nano-particles to the load-bearing capacity of tooth tissue — •Jean-Baptiste Forien[1], Claudia Fleck[2], Peter Fratzl[3], and Paul Zaslansky[1] — [1]Julius Wolff Institut, Berlin, Germany — [2]Technical University, Berlin, Germany — [3]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Teeth are hierarchical strong and stiff structures, consisting of a mineralized protein-based composite (dentine). They function under mechanical load, and the nanometer-sized hydroxyapatite mineral particles in the collagen fiber matrix deform as a response to applied external stress (Deymier-Black,2012). In this study, we report on the mineral response in human dentine to mechanical tensile testing. We track mineral particles following changes in the mineral dimension using X-ray diffraction. It is thus possible to compare the stresses experienced by the mineral particles with the stress applied by the external load. We find that the tissue to mineral strain ratios observed increase until they reach a value of 2, which is three times lower than for bone (Gupta,2006), and suggests that a different load-partitioning mechanism exists in teeth. We also find that the Poisson's ratio decreases with increasing load, suggesting that as load increases, there is some dynamic change in the loads transferred to the crystals, similar to what was found for bovine dentine loaded in compression. With increasing load, more strain-energy is orientated along the tensile axis and less is distributed into particles oriented along other orientations.

MM 38: Invited talk Maass

Time: Wednesday 15:00–15:30 Location: TC 006

Invited Talk MM 38.1 Wed 15:00 TC 006

Spatiotemporal deformation dynamics in metals — •Robert Maass — Georg-August-Universität Göttingen, Göttingen, Germany

Plastic deformation in metals proceeds intermittently in both space and time. In crystals these discrete processes are facilitated by collective dislocation rearrangements (dislocation avalanches), and in amorphous metals shear banding is the underlying process. In both cases the spatiotemporal nature of plastic flow is difficult to assess due to its spatial confinement to the nano-scale and the short time scales. In this talk we will present recent observations made during mechanical characterization that directly trace plastic instabilities, with the aim at approaching what ultimately controls the mechanical stability of structural metals. Both small scale crystals as well as amorphous metals are considered. We address slip size magnitude distributions, their involved time scales, and slip velocity distributions. We further discuss the appearance and disappearance of discrete plastic behavior, and combine the experimental results with insights from materials modeling to guide our micro structural understanding.

MM 39: Methods in Computational Materials Modelling V: Kinetics and Beyond DFT

Time: Wednesday 15:45–17:45 Location: H 0106

MM 39.1 Wed 15:45 H 0106

Exploring nucleation mechanisms in nickel: Novel insight from transition path sampling simulations. — •Grisell Diaz Leines, Ralf Drautz, and Jutta Rogal — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Universitätstr. 150, 44780 Bochum, Germany

Molecular dynamics simulations can provide valuable atomistic insight into solidification, but the modelling of the initial nucleation during solidification remains challenging due to the extended timescales of the process. Nowadays, advanced computational methods like transition path sampling (TPS) have enabled the investigation of nucleation on the atomistic level. In this work, we employ TPS to investigate the nucleation during solidification in nickel. We initially focus on homogeneous nucleation in elemental nickel as a function of undercooling. As a second step towards more complex materials, we extend our study by including small Ni-clusters as seeds during heterogeneous nucleation. The transition state ensemble obtained from our TPS simulations provides atomistic insight into the structure and size of critical nuclei for different nucleation mechanisms (homogeneous and heterogeneous nucleation at defects), as well as nucleation barriers/rates. Such results provide valuable information to validate and improve existing thermodynamic models describing nucleation. Furthermore, the information obtained about nucleation rates and the distribution of nucleation centres can also directly be connected to phase field models.

MM 39.2 Wed 16:00 H 0106

Annealing of coper nanoparticles on substrate by surface diffusion — •Raphael Schiedung[1], Ingo Steinbach[1], and Ulrich

Köhler[2] — [1]ICAMS, Bochum, Deutschland — [2]Ruhr Universität Bochum, Institute for Experimental Physics, Surface Physics, Bochum

Copper nanoparticles on zinc-oxide substrates are discussed as materials for heterogeneous catalysis. An electric field gradient at the contact line between particles, substrate and gas is a possible mechanism for the chemical activity of otherwise only chemically interactive materials. In processing of the nanoparticles an annealing step is employed after deposition on the substrate at moderate temperatures. Experimental studies revealed, that the nanoparticles are sightly sucked into the substrate during annealing that a small crater remains after removing individual particles. In order to reveal the mechanism and the dynamics of this process a phase-field study has been performed. Surface diffusion is assumed to be the underlying physical process for the structural changes of the nanoparticles on the surface. The multi-phase-field theory as implemented in the open-source software OpenPhase has been applied. It is based on the minimization of the free surface energies in the three phase system copper, zinc-oxide and gas. Results of the simulation are presented and compared to the experimental observations. This is a first step in theoretically investigating the multi-physics problem of deformation, piezoelectric activity of the substrate and electrostatic charging of the copper particles. Future work will concentrate the elastic and electric properties of the system in order to reveal the catalytic activity of the compound structure.

MM 39.3 Wed 16:15 H 0106

Simulation of fractal abnormal grain growth in nanocrystalline materials — •Mingyan Wang[1], Jules Dake[1], Rainer Birringer[2], and Carl Krill[1] — [1]Ulm University, Germany — [2]University of the Saarland, Germany

Despite an implicit rarity in its name, abnormal grain growth (AGG) appears to be a common mode of coarsening in nanocrystalline materials regardless of the specimen's composition or synthesis route. During AGG, a subpopulation of grains manifests rapid growth, leading to grain volumes that not only are much larger than those of their neighbors, but also are sometimes highly irregular in shape. The nature of this irregularity can be described by the geometric concept of fractals. This fractal morphology suggests that, in certain cases, AGG might proceed by some kind of percolation process along the "grid" defined by the initial ensemble of grains. We have investigated this possibility by extending a phase field algorithm for simulating grain growth to include selection rules for percolation. For properly chosen parameter values, the abnormal grains generated by simulation can be strikingly similar in shape to their experimental counterparts. Quantifying the comparison between simulation and experiment by fractal dimensionality, we hope to gain insight into at least one of the underlying physical mechanisms behind AGG in nanocrystalline materials.

MM 39.4 Wed 16:30 H 0106

On the Propagation of two en passent cracks upon mutual interaction: A pase field study — •Markus Thäter, Michael Fleck, 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 passent" 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 passent" 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 [1]: 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 alines 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.

15 min. break

MM 39.5 Wed 17:00 H 0106

Random phase approximation up to the melting point: The impact of anharmonicity and many-body effects on the thermodynamics of Au — Blazej Grabowski, •Stefan Wippermann, Albert Glensk, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Triggered by the Materials Genome Initiative the development of *ab initio* based materials databases has gained immense momentum. A crucial requirement is that the databases reliably provide quantitatively accurate data. However, the application of generalized-gradient corrected functionals within standard density-functional theory results in a dramatic failure for e. g. the heat capacity of Au, leading to divergent thermodynamic properties well below the melting point.

Here we present an extension of the upsampled thermodynamic integration using Langevin dynamics (UP-TILD) technique to compute accurate finite temperature properties including many-body effects. We employ the random phase approximation (RPA) within the adiabatic connection fluctuation dissipation (ACFD) framework, showing that the inclusion of many-body effects leads to a stabilization and to an excellent agreement with experiment. The study demonstrates the capabilities of the RPA – previously confined to T=0K – at finite temperatures.

MM 39.6 Wed 17:15 H 0106

Correlation energy in the Adiabatic Connection Fluctuation-Dissipation Theory beyond RPA: Systematic development and simple approximations — •Nicola Colonna[1], Maria Hellgren[2], and Stefano de Gironcoli[3,4] — [1]Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [3]International School for Advanced Studies (SISSA), I-34136 Trieste, Italy — [4]CNR-IOM Democritos, I-34136 Trieste, Italy

We present a systematic approach to compute accurate correlation energies in the adiabatic connection fluctuation dissipation (ACFD) framework beyond RPA. To first order our scheme leads to the RPA plus exact-exchange kernel (RPAx), for which a novel and efficient implementation is proposed. It is based on an eigenvalue decomposition of the time dependent response function of the Many Body system in the limit of vanishing coupling constant, evaluated by density functional perturbation theory. The accuracy of the RPAx approximation has been tested calculating the correlation energy of the homogeneous electron gas and studying the dissociation energy curves of selected diatomic molecules. A sensible improvement of the total energy description is disturbed by a pathological behavior of the response function. Staying within an exact first-order approximation to the response function, we use an alternative resummation of the higher-order terms. This slight redefinition of RPAx fixes the instability in total energy calculations without compromising the overall accuracy of the approach.

MM 39.7 Wed 17:30 H 0106

Comparison between exact and semilocal exchange potentials: An all-electron study for solids — •Fabien Tran[1], Markus Betzinger[2], Peter Blaha[1], and Stefan Blügel[2] — [1]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria — [2]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The exact-exchange (EXX) potential, which is obtained by solving the optimized-effective potential (OEP) equation, is compared to various approximate semilocal exchange potentials in selected solids (C, Si, BN, MgO, Cu_2O, and NiO). This is done in the framework of the linearized augmented plane-wave method, which allows for a very accurate all-electron solution of electronic structure problems in solids. In order to assess the ability of the semilocal potentials to approximate the EXX-OEP, we considered the EXX total energy, electronic structure, electric-field gradient, and magnetic moment. An attempt to parameterize a semilocal exchange potential is also reported.

MM 40: Nanomaterials II: Mechanical Properties

Time: Wednesday 15:45–18:00 Location: H 0107

MM 40.1 Wed 15:45 H 0107

Mechanical properties of Cu-Zr multi-composition nanoglasses — •Omar Adjaoud and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

Nanoglasses can be produced by consolidation of glassy nanoparticles which are prepared by inert-gas condensation. The microstructure of nanoglasses consists of glassy regions separated by glass-glass interfaces. These interfaces influence many properties of nanoglasses such as mechanical properties. It is know that the bulk metallic glasses with different composition response differently to the external load. In this work, we perform molecular dynamics simulations to address the question whether the composition of glassy nanoparticles could affect the mechanical properties of nanoglasses. we prepare multi-composition nanoglasses by compaction of several Cu-Zr glassy nanoparticles which have different composition. We discuss the behavior of the multi-composition nanoglasses during the mechanical tests in terms of local atomic strain and the atomic structure of the glassy nanoparticles forming the nanoglass.

MM 40.2 Wed 16:00 H 0107

Mechanical properties of Cu-Zr multi-composition nanoglasses — •Omar Adjaoud and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

Nanoglasses can be produced by consolidation of glassy nanoparticles which are prepared by inert-gas condensation. The microstructure of nanoglasses consists of glassy regions separated by glass-glass interfaces. These interfaces influence many properties of nanoglasses such as mechanical properties. It is know that the bulk metallic glasses with different composition response differently to the external load. In this work, we perform molecular dynamics simulations to address the question whether the composition of glassy nanoparticles could affect the mechanical properties of nanoglasses. we prepare multi-composition nanoglasses by compaction of several Cu-Zr glassy nanoparticles which have different composition. We discuss the behavior of the multi-composition nanoglasses during the mechanical tests in terms of local atomic strain and the atomic structure of the glassy nanoparticles forming the nanoglass.

MM 40.3 Wed 16:15 H 0107

Aspects of universal yield behavior of bulk metallic glasses unraveled in nanocrystalline Pd-Au alloys — •Andreas Leibner, Christian Braun, Jonas Heppe, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, FR7.2 Experimentalphysik, Campus D2 2, 66123 Saarbrücken

We present experimental evidence that plastic yielding of nanocrystalline (NC) metals at the low end of the nanoscale is reminiscent of universal yield behavior of metallic glasses. NC Pd-Au samples with a grain size of $D \lesssim 10\,\mathrm{nm}$ and isotropic microstructure were deformed under different conditions: From strain-rate dependent deformation studies on shear-compression-specimens, we find that the energy barrier height of NC Pd_{90}-Au_{10} exhibits universal scaling behavior $\Delta G \propto \Delta\tau^{3/2}$ [1], where $\Delta\tau$ is a residual load, giving rise to a generalization of the Johnson-Samwer $T^{2/3}$ scaling law [2] of yielding in metallic glasses. Additionally, we use microhardness as measure for the shear yield stress of Pd-Au samples with different Au-concentrations (and concomitantly different elastic moduli). As a result, the NC alloys exhibit the linear correlation $\tau_y/G = 0.00267 \pm 0.002$ discovered for over 30 bulk metallic glasses [2]. Since shear transformations are considered to be the generic flow defect in metallic glasses, it seems reasonable to suppose that shear softening of grain boundaries provokes the occurrence of shear transformations.

[1] M. Grewer and R. Birringer, PRB **89**, 184108 (2014)
[2] W.L. Johnson and K. Samwer, PRL **95**, 195501 (2005)

MM 40.4 Wed 16:30 H 0107

An analysis of thermal activation parameters in nanocrystalline metals — •Anja Steinbach, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

We studied the plasticity of thermally equilibrated and non-equilibrated nanocrystalline (NC) $Pd_{90}Au_{10}$ samples with grain sizes below 10 nm by using the miniaturized shear compression specimen (m-SCS) [1]. We performed strain-rate and temperature-dependent mechanical tests under dominant shear and superimposed compression up to large plastic strains to deduce the shear activation volume Δv, strain-rate sensitivity m, as well as the Gibbs free energy of activation ΔG. These thermal activation parameters are most informative for probing the mechanisms of thermally activated plasticity [2].

[1] M. Ames, J. Markmann, R. Birringer, Mater. Sci. Eng. A 528, 526 (2010)
[2] M. Grewer, and R. Birringer, Phys. Rev. B 89, 184108 (2014)

15 min. break

MM 40.5 Wed 17:00 H 0107

X-ray nanodiffraction meets materials science — •Christina Krywka[1], Stephan Roth[2], and Müller Martin[1] — [1]Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, Geesthacht D-21502 — [2]DESY, Notkestraße 85, Hamburg D-22607

The Nanofocus Endstation of beamline P03 (PETRA III, Hamburg) is operated jointly by Helmholtz Zentrum Geesthacht and the University of Kiel, and is one of the very few synchrotron endstations providing the experimental conditions for scanning X-ray nanodiffraction. This technique, in turn, is an excellent tool for materials science. It readily serves structural information with sub-micrometer spatial resolution from crystalline and semi-crystalline materials (metals, biomaterials, synthetic compounds) for the retrieval of e.g. grain orientation, residual stress profiles, crystal structure or texture. Because of the long focal distance focusing, the wide energy range of the P03 beamline and a hexapod based positioning system, high resolution nanodiffraction experiments can be performed on strongly absorbing metallic samples and in extended sample environments, using a beam with a size of only 350 nm * 250 nm, generated using a long focal distance focusing system.

The strong focus on materials science at P03 is demonstrated by the wide range of experiments already performed with in situ sample environments: pressure, indentation force, tensile stress, fluid shear, magnetic fields - all of these parameters were successfully modified in situ and combined with the high spatial resolution provided by nanofocused beam.

MM 40.6 Wed 17:15 H 0107

Tunable magnetic anisotropy in elongated Ni nanoparticles embedded in SiO2 matrix by swift heavy ions irradiation — •Debalaya Sarker, Santanu Ghosh, and Pankaj Srivastava — Department of Physics, Indian Institute of Technology Delhi

The discovery of nanoparticle elongation inside insulator matrix by swift heavy ion (SHI) irradiation and its association to thermal spike model has led to interest in different physical properties of such systems. The ease of switching the easy axis of magnetization by elongating embedded ferromagnetic Ni nanoparticles in insulator matrix by SHI bombardment in the direction of incident beam, has motivated the present study. Ni foils glued on SiO2 target were co-sputtered. Irradiation with 100 MeV Au+7 SHI was carried out at different fluences. GISAXS analysis confirms elongation of NPs along beam direction but along with an overall volume reduction. In-plane and out-plane M-H measurements at 5 K show that gradual increase in saturation magnetization and coercivity till 5.0*1013 ions/cm2 fluence. XANES and valence band XPS show narrowest 3d electron-band for the same, resulting in maximum spin polarization. We conclude that at further higher fluences dissolution of NPs have caused overall volume reduction and hence results in reduction of shape anisotropy originated perpendicular magnetization. Thus the intermediated fluence irradiated film, having the maximum out of plane magnetization, can find its promising applications in future perpendicular magnetic storage devices capable of thrice storage capacity in comparison to normal linear storage media.

MM 40.7 Wed 17:30 H 0107

Synthesis and Properties of Solids Composed of Organic-

Linked Nanoparticles — •Axel Dreyer[1], Artur Feld[2], Ezgi D. Yilmaz[1], Wolfgang Heckel[1], Stefan Müller[1], Horst Weller[2], and Gerold A. Schneider[1] — [1]Hamburg University of Technology, Institute Advanced Ceramics, Hamburg, Germany — [2]Hamburg University, Institute of Physical Chemistry, Hamburg, Germany

Natural hard tissues like nacre or enamel are characterized by outstanding mechanical properties in relation to their rather weak mechanical constituents. They key of their mechanical behavior is the combination of hard inorganic and soft organic constituents in a hierarchical structure, which starts on the nanoscale. Our approach is an attempt to synthesize the first hierarchical level by the self-organization of organic-coated nanoparticles into close-packed superstructures. The organic molecules play a prominent role by providing cohesion in the material via strong coordinated binding of functional groups to the inorganic particles as well as weak van der Waals binding between adjacent molecules. We present the successful manufacturing of extensive nano-particle superstructures by a sequence of sedimentation, drying, heating, and pressing of monodispersed spherical iron oxide particles. In a subsequent step we will increase the interparticle binding energy by controlled chemical crosslinking within the organic shell of the solid particle superstructures. The mechanical properties of these nano-composites like hardness, elastic modulus, and strength will be discussed and related to the binding energy in the interparticle space.

MM 40.8 Wed 17:45 H 0107

Bilayer Gold Nanostructures for Optical Activity in the Visible Range — •Katja Höflich[1,2], Gaudhaman Jeevanandam[2], Julia Schneider[2], Caspar Haverkamp[1,2], and Silke Christiansen[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin — [2]Max-Planck-Institut für die Physik des Lichts, Günther-Scharowsky-Str. 1, 91058 Erlangen

Tailored manipulating of light onto the nanoscale is key for any nano-optical application. Especially, turning the polarization vector of mostly circularly polarized light by so-called optically active nanostructures created huge interest in the in the fast-growing field of plasmonics and metamaterials. Here we present optical activity in the visible range for chiral nanostructures combining positive with the corresponding negative L-shapes in a bilayer system with strong near-field coupling through a silicon dioxide membrane. Using electromagnetic modeling (finite difference time domain) the structures were optimized with respect to small ellipticity (defining the deformations of the incident circular polarization state) while guaranteeing large optical activity. The fabrication is based on focused ion beam milling of single-crystalline gold flakes and dedicated nano-manipulation, spectroscopic characterization was carried out in a fiber-coupled optical microscope equipped with a Horiba spectrometer.

MM 41: Electron Microscopy

Time: Wednesday 15:45–17:15 Location: TC 006

MM 41.1 Wed 15:45 TC 006

Five-fold dissociation of dislocations in the hexagonal complex metallic alloy my-AlMn — •Marc Heggen, Stefan Roitsch, and Michael Feuerbacher — Ernst Ruska Centrum, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

Complex metallic alloys (CMAs) are a class of intermetallics characterized by a high structural complexity, large lattice parameters, and a multitude of atoms per unit cells. In recent years, novel complex defects and new mechanisms of plastic deformation have been reported in these alloys. In this contribution defects in the CMA my-AlMn, a hexagonal phase (space group P63/mmc) with 563 atoms per unit cell and lattice parameters a=2.0 nm and c=2.5 nm are investigated. Using state-of-the-art aberration-corrected scanning transmission electron microscopy, the atomic dislocation and stacking fault structure is studied in plastically deformed my-phase samples. We demonstrate the existence of groups of five dissociated dislocations, having [0 0 1] line direction. The dislocations are partials connected by complex stacking faults with typical overall splitting distance of 100 nm employing two different types of hexagonal structural subunits.

MM 41.2 Wed 16:00 TC 006

Effect of severe plastic deformation on Al3Sc precipitation in an Al-Mg-Mn-Sc alloy — •Yulia Buranova[1], Anna Mogucheva[2], Harald Rösner[1], Ankit Gupta[3], Tilmann Hickel[3], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — [2]Belgorod State University, 85 Pobedy, 308015 Belgorod, Russia — [3]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Aluminum alloys containing scandium show excellent mechanical properties due to the presence of Al3Sc precipitates. In this study the effect of severe plastic deformation using equal channel angular pressing (ECAP) on the formation of Al3Sc precipitates has been investigated. The grain size, dislocation density, particles size, chemistry and particle distribution were investigated by analytical transmission electron microscopy. Additionally, geometric phase analysis (GPA) was applied to map local strains. The chemical mapping reveals a uniform distribution of Mg in the Al matrix. Three types of precipitates are generally found. The smallest particles, mostly Al3Sc, are coherent with sizes of 5-10 nm. Precipitates around 15-30 nm are found to contain Al, Mg, Mn and Sc. Larger particles contain mainly Al and Mn. These chemical trends are compared with ab initio calculations. While the middle- and large-size precipitates are predominantly found along grain boundaries and dislocation lines in their initial state, the ECAP processing produces an almost uniform distribution of particles. The experimental findings are compared with predictions based on atomistic simulations.

MM 41.3 Wed 16:15 TC 006

Comprehensive model of metadislocation motion in o-$Al_{13}Co_4$ — •Markus Heidelmann, Marc Heggen, Christian Dwyer, and Michael Feuerbacher — Ernst-Ruska-Centrum, Forschungszentrum Jülich, 52425 Jülich, Deutschland

In several complex metallic alloys plastic deformation is mediated by metadislocations. Due to the complex nature of these defects and the large number of atoms in their core region, little is known about the atomic rearrangements taking place during movement of a metadislocation. In this work we report on the first development of a fully three-dimensional model of a moving metadislocation including all atomic species. The CMA chosen for our study is the moderately complex o-$Al_{13}Co_4$, an orthorhombic phase with 102 atoms per unit cell. Using a combination of high-resolution scanning transmission electron microscopy and density functional theory, we have developed an atomic model for the [010] glide movement of a metadislocation in $Al_{13}Co_4$ extending to light elements and including the third dimension. Metadislocation movement was analysed employing a simulated-annealing procedure to minimize the total jump distance of all atoms within the model. While the distance of one glide step is 12.3 Å, the maximum jump distance of an individual atom is a much more moderate 3.4 Å. The approach described is versatile enough to be applied to other, more complex problems, for example metadislocation movement in ϵ_6-Al-Pd-Mn.

We kindly acknowledge funding from the DFG under project Pak 36 / FE 571/2-2.

MM 41.4 Wed 16:30 TC 006

Crystallization of amorphous FeNiP nanowire arrays studied by in-situ TEM — Nina Winkler, •Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, Westfälische-Wilhelms-Universität Münster, NRW

Nano-scaled magnetic materials are in focus of basis research since decades, and of remarkable technical importance. In this work, an array of amorphous soft magnetic nanowires was successfully processed using porous Anodic Alumina Oxide (AAO) templates. This enables to study the crystallization in confined volumes and to control the regularity and shape of the nanostructures via the AAO pores which are uniform in length and diameter. Fe40Ni40P20 (at. %) nanowire arrays were processed into the AAO pores by electrodeposition. Differential scanning calorimetry (DSC) of a likewise processed thin film shows a glass transition. Upon in-situ annealing in the transmission

electron microscope (TEM) the microstructural evolution can be detected. Crystallization kinetics includes long range diffusion and a high nucleation rate. Annealing at temperatures above the crystallization temperature follows a phase separation of FeNiP in multilayers of FeNi and FeNiP phases. The impact of different heating rates on the phase evolution is studied by DSC. The obtained magnetic properties are characterized by a Vibrating Sample Magnetometer (VSM).

MM 41.5 Wed 16:45 TC 006

Determination of local density in amorphous materials based on HAADF-STEM signals — •Lea Kümper[1], Vitalij Schmidt[1], Harald Rösner[1], Martin Peterlechner[1], Tobias Brink[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

It was shown that in metallic glasses narrow zones with different densities in comparison to the surrounding matrix are formed during plastic deformation. These deformation zones are called shear bands. Using high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) it is possible to quantify the local density changes in amorphous materials and thus in shear bands [1]. The quantification of the local density change ρ was based on the approximation that the density change can be calculated according to: $\Delta\rho = \frac{\rho_1-\rho_2}{\rho_2} \cong \frac{I_1 x_k^1 t_2}{I_2 x_k^2 t_1} - 1$, where ρ is the density, x_k is the contrast thickness and t is the foil thickness for different zones in a sample. In this contribution the reliability of this approximation is investigated experimentally using amorphous Si-Ge multilayer systems as calibration standards. Additionally, we obtained Cu-Zr glass structures with shear bands by molecular dynamics computer simulations. These were used to obtain the corresponding HAADF-STEM images via image simulation. The obtained results are discussed with respect of the accuracy of the density determination method. [1] H. Rösner et al., Ultramicroscopy, 142 (2014)

MM 41.6 Wed 17:00 TC 006

Comparison of medium-range order in shear bands and matrix of a metallic glass by fluctuation electron microscopy — •Vitalij Schmidt[1], Harald Rösner[1], Martin Peterlechner[1], Paul Voyles[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Materials Science and Engineering, University of Wisconsin-Madison, 1509 University Ave, Madison, WI53706, USA

The deformation behavior of metallic glasses is yet not fully understood. For temperatures well below the glass transition and high strains the plastic flow is restricted to narrow areas called shear bands while the surrounding amorphous matrix seems unaffected. Thus modifications of the local medium-range order (MRO) are likely to be expected in the shear bands. In order to analyze the structural modifications in shear bands directly, melt-spun and subsequently cold-rolled $Al_{88}Y_7Fe_5$ ribbons were selected and prepared for transmission electron microscopy (TEM) by electro-polishing. The thin foils exhibit shear bands with contrast changes along their propagation direction observed by high-angle annular dark-field (HAADF)-STEM. Fluctuation electron microscopy has been used to characterize the deformed metallic glass samples by analyzing sets of nanobeam-diffraction patterns. Azimuthal profiles are extracted from the variance of these sets resulting in a measure for the MRO. Different parts of the observed shear bands are compared with the surrounding matrix showing differences in MRO with respect to the contrast changes.

MM 42: Mechanical Properties I

Time: Wednesday 15:45–18:00 Location: TC 010

MM 42.1 Wed 15:45 TC 010

A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron — •Mira Todorova[1], Klaus-Dieter Bauer[2], Kurt Hingerl[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Zentrum für Oberflächen- und Nanoanalytic, Universität Linz, Altenberger Str. 69, 4040 Linz, Austria

Using density-functional theory calculations we study the embrittling behaviour of liquid Zn in the $\Sigma3[111]60°$ and the $\Sigma5[100]36.8°$ symmetric tilt grain boundaries in bcc iron (ferrite). Investigating Zn induced changes in the energetics of the grain boundaries and their associated free surfaces we utilise both the canonical Griffith model and the grand canonical Rice-Wang formulation to evaluate the difference between the calculated grain boundary energies and the surface energies of their corresponding surfaces. We find that Zn wetting can reduce the cohesive strength of the interface by up to 40% and that the critical nominal bulk Zn concentration at which grain boundary weakening starts is almost two orders of magnitude lower in a grand-canonical model compared to the canonical case. The obtained results will be critically reviewed and discussed in the context of the embrittling behaviour of liquid zinc.

K.-D. Bauer, M. Todorova, K. Hingerl and J. Neugebauer, Acta Materialia (submitted).

MM 42.2 Wed 16:00 TC 010

Absorption of dislocations in grain boundaries: atomic scale information for mesoscale models — •Julien Guénolé, Aruna Prakash, and Erik Bitzek — Department of Materials Science an Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Dislocation-grain boundary (GB) interactions play an important role in the plastic deformation of polycrystalline materials, in particular for nanocrystalline metals. Advanced models for the mechanical behavior of nanocrystalline metals therefore need to take GBs explicitly into account. Several approaches to include GBs into mesoscale models (dislocation dynamics, strain gradient plasticity models, ...) were recently suggested. Such GB models need information, like the conditions for dislocation absorption, the change of dislocation stress fields after absorption, or on how much dislocation content can be absorbed. Atomistic simulations are uniquely positioned to provide such information and advance our understanding on dislocation-GB interactions.

Here we present results of carefully controlled studies of dislocations interacting with GBs in model bicrystalline samples. The mechanisms during dislocation-GB interaction are studied in quasi-2D and fully 3D samples. The stress and energetic signatures of the absorbed dislocations are analyzed and a novel approach to model the effect of the dislocation absorption on the dislocation stress field is proposed. A primary aim of the current study is to provide a better understanding of the role of absorbed dislocation content in the GB on the pinning and nucleation of other dislocations.

MM 42.3 Wed 16:15 TC 010

Atomistic Simulations of Dislocation-Interface Interactions in the γ/γ' Microstructure in Ni-base Superalloys — •Aruna Prakash, Julien Guénolé, Juan Wang, and Erik Bitzek — Materials Science and Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Single crystal Ni-base superalloys are characterized by an ordered $L1_2$ γ'-phase (comprising mostly of Ni_3Al) that precipitates as cuboidal particles in the face centered cubic (fcc) γ-channels comprising mainly of Ni. The interaction of dislocations in the channels with γ' precipitates plays an important role for the high-temperature mechanical properties of Ni-base superalloys. To date, most atomistic simulations concerning dislocation interface interactions in such materials have been performed with simplistic quasi-2D geometries. Here we report on simulations performed with a full 3D setup obtained by a novel approach that facilitates the reconstruction of experimental microstructures obtained from atom probe tomography. The reconstructed sample allows us to study the interaction of the relevant dislocations (screw and 60 degree) with a realistic curved interphase boundary, both in samples with ideal stoichiometric chemical composition and with concentration gradients of specific atoms. Static calculations as well as molecular dynamic calculations were performed to determine the interaction of the channel dislocations with the misfit dislocation network. The results of the simulations with the above setup are compared with those from a canonical quasi 2D approach and a 3D model and are discussed in the framework of a multiscale approach.

MM 42.4 Wed 16:30 TC 010

Modeling nanoporous gold: on the influence of nodal shifting and ligament size distribution — •Bao-Nam D. Ngô[1,2], Alexander Stukowski[2], Jürgen Markmann[1,3], Karsten Albe[2], and Jörg Weissmüller[1,3] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Darmstadt, Germany — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

We present a study of the influence of topology on mechanical behavior of nanoporous gold – a promising material for applications in actuation, catalysis and sensing, as well as a model candidate for study of plasticity at nanoscale. Using molecular dynamics, two topological descriptors were investigated: nodal shifting and ligament diameter distribution. For that purpose, we first studied a highly symmetric diamond-like structure – an idealized structure proposed recently by Finite Element Modeling. Then we gradually altered the topology of this symmetric structure in two different directions: randomly displacing its nodal positions and changing its ligament diameter distribution. Relevant mechanical properties investigated include macroscopic stress-strain behavior, deformation-induced structural changes, evolution of effective Young's modulus, and evolution of defect densities. Our results show that both topological descriptors are important and strongly affect the mechanical properties of nanoporous gold.

15 min. break

MM 42.5 Wed 17:00 TC 010

Refined statistical work hardening and recovery model for Aluminium alloys — •Volker Mohles[1], Volker Pankoke[1], Philipp Schumacher[2], and Benjamin Milkereit[2] — [1]RWTH Aachen University, Institute of Physical Metallurgy and Metal Physics, Aachen, Germany — [2]University of Rostock, Chair of Materials Science, Rostock, Germany

A new statistical work hardening and recovery model for aluminium alloys called 4IVM (4 Internal Variables Model) has been developed. Like its established predecessor (3IVM+) it calculates the evolution of dislocation densities during plastic deformation and derives the corresponding flow curves in a wide range of temperatures and strain rates. In order to improve the physical basis and its applicability, the new model considers four densities of dislocations as material state variables: mobile dislocations (ρ_{mob}), dipole dislocations (ρ_{dip}), locked dislocations (ρ_{lock}), and subgrain boundary dislocations (ρ_{sub}). These dislocation types have distinctly different properties, in reality and in the model, with respect to generation, annihilation, direct impact on the flow stress, and the overall dislocation density evolution. Moreover their cores and strain fields differ. In future this allows to introduce specific dependencies on segregation by foreign solved atoms. The new model is validated by comparing simulated flow curves to measured ones. For this, binary Al-Si alloys have been prepared and compression tested in varying precipitation states. Compared to its predecessor, 4IVM offers improved flow curve predictions.

MM 42.6 Wed 17:15 TC 010

Work hardening of Cu based conductors by deformation under cryogenic conditions — •Jens Freudenberger[1], Felix Thiel[1,2], Alexander Kauffmann[1,3], and David Rafaja[2] — [1]IFW Dresden — [2]TU Bergakademie Freiberg — [3]KIT

Cu-Ag-Zr alloys show a beneficial combination of high mechanical strength and good electrical conductivity making these materials suitable for a variety of applications, which strongly rely on this combination of properties. The mechanical as well as electrical properties of Cu-Ag-Zr alloys are strictly related to their microstructure, which can be adjusted by manufacturing processes. This study shows the effect of cryogenic wire drawing of dynamically recrystallized Cu-Ag7-Zr0.3 alloys on its microstructure in comparison to material which has been deformed at room temperature. The different microstructural features such as grain size, dislocation density as well as precipitate size and their morphology were assessed. In addition, the formation of mechanical twins during cryogenic deformation is reflected. The mechanical and electrical properties of the alloy are explained upon the observed microstructure.

MM 42.7 Wed 17:30 TC 010

Deformation mechanisms of nano-twinned Ag wires and Cu — •Aaron Kobler[1,2], Thorsten Beuth[1], Markus Moosmann[1], Thomas Schimmel[1], Horst Hahn[1,2], and christian Kübel[1,3] — [1]Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Technische Universität Darmstadt (TUD), Jovanka-Bontschits-Straße 2, 64287 Darmstadt, Germany — [3]Karlsruhe Nano Micro Facility (KNMF), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Introducing nanotwins into the material is one possible approach to increase ductility and achieve high strength. However, the deformation mechanisms that govern the high strength and high ductility are still unresolved as twin boundaries can act as both barriers and sources for dislocations. For the materials strength, twin boundaries play a similar role as grain boundaries in ufg and nc metals, i.e. decreasing the twin spacing generally results in increased strength. We present Ag nanowires with twin planes parallel to the <112> wire axis. Using indentation experiments, we investigated the deformation mechanisms of individual nanowires. Further, we present in-situ tensile tests inside the TEM in combination with orientation mapping of nanotwinned Cu. In both cases we see a clear orientation dependent plastic deformation that we will analyze with respect to the underlying mechanisms.

MM 42.8 Wed 17:45 TC 010

Influence of alloying elements on the fracture strength of iron — •Sankari Sampath and Rebecca Janisch — ICAMS, Ruhr Universität Bochum, 44780 Bochum

Studying crack nucleation is the first step of understanding the fracture behavior of a material. With ab-initio density-functional theory calculations of fracture strength we identify possible nucleation sites for brittle cracks. In ferritic iron potential candidates are the well known {001} cleavage planes as well as different interfaces in the microstructure. The strength of both can change considerably with impurity or alloying element content, in our case silicon and carbon. Detailed studies on the strengthening effect of C on the interface structures and the embrittling nature of Si at the grain boundaries are available. In this work, the co-doping effects of both Si and C are of special interest. To identify the weakest type of interface or cleavage plane, and to investigate the influence of alloying elements on its strength, different model structures were created. The energy of formation of interstitial C in the single crystal as well as at the interfaces in the presence or absence of Si gives an insight on the expected composition of grain boundaries in Fe-Si-C alloys. The subsequent calculations of fracture strength with one or both type of elements reveal interesting non-linear effects.

MM 43: Invited talk Kaplan

Time: Wednesday 18:30–19:00 Location: TC 006

Invited Talk MM 43.1 Wed 18:30 TC 006
Structural vs Chemical Adsorption Transitions at Surfaces & Interfaces — •Wayne Kaplan — Department of Materials Science & Engineering, Technion - Israel Institute of Technology, Haifa, Israel

It is recognized that grain boundaries (GBs) can be described using diffuse interface theory, where the structure and chemistry of GBs, interfaces and surfaces can go through 2-D transitions between thermodynamic states (termed complexions) in order to minimize the interface energy. As such, complexions for surfaces and interfaces are analogous to phases in the bulk. To date, almost all studies have been conducted on GBs in single phase polycrystalline systems, which by definition are not at equilibrium. Similar questions have been raised regarding interfaces in thin film studies, where the deposition process may be very far from equilibrium.

This presentation will focus on an experimental approach to address the structure, chemistry, and energy of complexions at interfaces which are fully equilibrated, from which it can be demonstrated that a change in complexion minimizes interface energy. This will be compared with solid-liquid interfaces, where a region of ordered liquid exists adjacent to the interface at equilibrium, and the details of a solid-solid interface where the reconstructed interface structure accommodates lattice mismatch for a nominally incoherent interface. These three systems will be compared to known reconstructed solid surfaces, which can also be described as complexions, within a more generalized Gibbs adsorption isotherm.

MM 44: Invited talk Rogal

Time: Wednesday 19:00–19:30 Location: TC 006

Invited Talk MM 44.1 Wed 19:00 TC 006
Modelling solid-solid phase transformations: Atomistic insight on mechanisms and interface properties — •Jutta Rogal — Ruhr-Universität Bochum, Bochum, Germany

Atomistic modelling of the dynamics of phase transformations is a particularly challenging task. If the mechanism of the phase transformation is governed by so-called rare events then the time scale of interest will reach far beyond the capabilities of regular molecular dynamics simulations.

The atomistic rearrangements during solid-solid phase transformations in bulk systems involve massive structural changes including concerted multi-atom processes. The interface between two structurally different phases leads to a complex energy landscape that needs to be explored during the dynamical evolution of the interface. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach to investigate such processes at the interface between cubic and topologically close-packed phases in transition metals.

In particular we investigate the transformation between BCC and A15 in molybdenum. During the dynamical simulations a finite, disordered interface region evolves to compensate the structural mismatch between the two crystal phases. This disordered interface region makes the identification of a single transformation mechanism difficult. Still, from our simulations we extract a rate for the layer transformation which we relate to an effective barrier for the transformation mechanism and discuss the corresponding atomistic processes that we find along the transformation path.

MM 45: General Meeting of the Metal- and Materials Physics Division and Presentation of the Best Poster Award

Time: Wednesday 20:00–21:00 Location: TC 006

Mitgliederversammlung

MM 46: Focused Session on GHz Dielectrics: Materials for Mobile Communication I (jointly with HL, MM, DY)

The world wide amount of wireless data exchange doubles roughly every year. In addition the individual data rates increase and the efficiency of the data exchange needs improvements. Antenna and filter elements are key components for such a development and are subject to intense research efforts. Impulses for innovation also originate from materials while new antenna and filter concepts influence material development. Two Focused Sessions are addressing the subject.

Organizer: Martin Letz (Schott AG Mainz)

Time: Thursday 9:30–13:00 Location: EB 407

Topical Talk MM 46.1 Thu 9:30 EB 407
New application scenarios for dielectric materials in mobile communication systems of the 5th generation — •Roland Gabriel — Kathrein-Werke KG, Anton-Kathrein-Straße 1-3, D-83004 Rosenheim / Germany

The worldwide data volume in mobile communication systems double nearly every year. To address this challenge, higher frequency bands will be used and broadband and multiband equipment are required. The new standard LTE-A and the standardization process for the 5th generation of the mobile communication systems enforces changes in the technology of antennas and filters. Beside the usage of new and higher frequency bands up to 60 GHz the broadband and multiband approach increase the requirements for the linearity of the components. For the use in FDD (frequency division duplexing) - systems this means an extreme low level of the active and passive intermodulation. In this contribution the extendend requirements for passive intermodulation are discussed. Different available solutions for the filter technology will be compared regarding the usage for different system solutions of the 4th and 5th generation. In addition the use of dielectric radiators in antennas will be reconsidered with respect to the multiband approach and the required inter- and intra-band isolation.

MM 46.2 Thu 10:00 EB 407
Impedance matching for high power transistors based on printed ceramics — •Alex Wiens, Daniel Kienemund, and Rolf Jakoby — Technische Universität Darmstadt, Institut für Mikrowellentechnik und Photonik

The multitude of standards in modern tele-communication systems,

such as GSM, UMTS, LTE and WiFi make the hardware of a radio front end face a variety of frequencies and bands. Generally, each element of the front end is optimized to perform best at a certain frequency band and signal type. Power amplifiers can be considered as the most critical components of RF/microwave communication systems, as they dominate the power consumption and hence the efficiency of the whole system. They are therefore consequently the focus of intense research to achieve improved linearity and increased power efficiency. Barium-Strontium-Titanate (BST) varactors offer an alternative to semiconductor and MEMS technologies in the design of tunable matching networks for reconfigurable multi-band RF-power amplifiers, and for load modulation applications, where the varactor tuning is used to maintain high efficiency over a large dynamic range of the input signal. Recent advances in fabrication of high power tunable RF varactors based on BST are presented and discussed. Measurement results of a BST-based tunable matching network, implemented inside a GaN HEM Transistor show promissing performance for telecommuncation frequency range.

MM 46.3 Thu 10:20 EB 407

Enhanced magnetooptic Kerr effect and magnetic properties of Ce:YIG thin films — •Andreas Kehlberger[1], Kornel Richter[1], Gerhard Jakob[1], Mehmet C. Onbasli[2], Gerald F. Dionne[2], Dong Hun Kim[2], Taichi Goto[2], Gerhard Götz[3], Günter Reiss[3], Timo Kuschel[3], Caroline A. Ross[2], and Mathias Kläui[1] — [1]Universität Mainz, Mainz, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]CSMD, Physics Department, Bielefeld University, Germany

Yttrium iron garnet (YIG) is a ferrimagnetic and electrically insulating garnet oxide that has low intrinsic magnetic damping. These properties make YIG a functional layer for spin-wave generation and filtering for telecommunication devices operating at microwave bands. The substitution of Y by Ce allows for an enhancement of the magnetooptic properties and to further influence the magnetic material properties. Our work presents an extensive study of high quality epitaxial Ce:YIG thin films and reveals that not only the magnetooptic properties but also the magnetic anisotropy can be tailored by the Ce substitution. For the first time we show that beside the Faraday rotation also the magnetooptic Kerr effect is enhanced compared to pure YIG, making a broader range of wavelength, including the fibreoptics band, accessible. We present growth methods for polycrystalline Ce:YIG films, which allow the development of integrated on-ship devices.[1,2] Our results show the suitability of Ce:YIG thin film for future magnetooptic and spintronic applications. [1] Lei Bi et al., Nature Photon. 5, 758-762 (2011) [2] Taichi Goto et al., J. Appl. Phys. 113, 17A939 (2013)

MM 46.4 Thu 10:40 EB 407

Design of miniaturized antennas for GNSS applications using a high DK dielectric material — •Stefano Caizzone — Institute of Communications and Navigation, German Aerospace Center (DLR), Wessling, Germany

The use of high dielectric constant (high DK) materials is particularly appealing for a vast number of Radio Frequency (RF) applications, including antenna design. In this field, in fact, high DK low-loss dielectric materials could enable consistent improvements in antenna miniaturization. To the present day, however, common high-DK materials suffer from relatively large manufacturing tolerances, implying remarkable frequency shifts in the antenna radiation and need for retuning. This work, on the other hand, shows the use of a new dielectric material with diminished tolerances for antenna design purposes, both through preliminary tests with a simple antenna structure and through the enhanced design of a miniaturized antenna for GNSS applications. The initial tests were performed in order to validate the usability of the material in the RF area: it was used as a substrate for a microstrip patch antenna. The results show a good behavior of the high DK material and its aptitude for RF antenna design. As a consequence, a Dielectric Resonator Antenna (DRA), fully exploiting the dielectric properties of the material, was designed for use in the lower L-Band of the Global Navigation Systems, allowing for good performance over a wide bandwidth, covering E5, L2 and E6 bands.

Topical Talk MM 46.5 Thu 11:00 EB 407

Dielectric-loaded antennas for circular polarisation: their contribution to the information capacity of wireless terminals — •Oliver Leisten — Maruwa Europe Ltd, UK

Dielectric-loaded multi-filar helix antennas offer solutions as miniature circular polarised antennas in small devices with the advantage that body-loading can suppress reflections from the device: improving circular polarisation discrimination. This is an example of materials-science enabling the design of antennas providing relatively predictable performance in a cluttered and changing near environment. Modern wireless systems typically operate with complex scattering from objects in the indoor environment which can be scaled in frequency to be compared to the Rayleigh scattering of light from the particles of dense smoke. Indeed modern MIMO devices exploit the low spatial autocorrelation of such fields invoking the principle of spatial multiplexing to multiply the information capacity per unit of spectral bandwidth. Such systems use multiple receiving antennas to receive scattered signals summing by superposition, at those discrete antenna locations, of information streams transmitted from multiple transmitting antennas. The small resonance volume dielectric-loaded antennas, together with platform independent polarisation, enhances statistical independence of signals, improving system data-capacity by reducing interference between data-streams. The use of right and left hand circular polarised antennas to invoke polarisation diversity is interesting as Rayleigh scattering develops spin-turbulent fields.

20 min Coffee Break

MM 46.6 Thu 11:50 EB 407

$Ba_4Al_2Ti_{10}O_{27}$ glass-ceramics as dielectric materials for antenna elements in wireless communications — •Martun Hovhannisyan[1], Hubertus Brauna[1], Yuliang Zheng[2], Arshad Mehmood[2], Martin Letz[1], and Rolf Jakoby[2] — [1]Material & Technology Development, SCHOTT AG, Hattenbergstrasse 10, Mainz, 55122, Germany — [2]Technical University of Darmstadt, Darmstadt, D-64283 Darmstadt, Germany

Dielectric glass-ceramics with $Ba_4Al_2Ti_{10}O_{27}$ as the main crystalline phase are obtained by controlled heat-treatment of a non-porous bulk-glass phase. Such a non-porous material has advantages over ceramics with residual porosity wherever metallization steps are applied to the material. Depending on the details of heat-treatment profile the $Ba_4Al_2Ti_{10}O_{27}$ is formed as a main phase with secondary phases $BaTi_4O_9$ or $BaAl_2Si_2O_8$. Microstructural observation using scanning electron microscopy (SEM) shows nanometer-sized crystals (40nm) grown in a true glass phase. The microwave dielectric characterization using Hakki-Coleman setup shows a Qf from 2000 GHz to 10.000 GHz, dielectric constant from 19 to 33 and |tf| of $<$20 ppm/K. Balancing between different crystalline phases allows to adjust |tf| to zero. To our knowledge the present work is the first one emphasizing the attractiveness of the microwave dielectric properties of the phase $Ba_4Ti_{10}Al_2O_{27}$. Such glass-ceramics are well suited for antenna and filter applications in microwave electronics.

MM 46.7 Thu 12:10 EB 407

Highly conducting $SrMoO_3$ thin films for microwave applications — •Aldin Radetinac[1], Arzhang Mani[1], Sergiy Melnyk[2], Mohammad Nikfalazar[2], Jürgen Ziegler[1], Yuliang Zheng[2], Rolf Jakoby[2], Lambert Alff[1], and Philipp Komissinskiy[1] — [1]Institute for Materials Science, TU Darmstadt, Germany — [2]Institute for Microwave Engineering and Photonics, TU Darmstadt, Germany

We have measured the microwave resistance of highly conducting perovskite oxide $SrMoO_3$ thin film coplanar waveguides. The epitaxial $SrMoO_3$ thin films were grown by pulsed laser deposition and showed low mosaicity and smooth surfaces with a root mean square roughness below 0.3 nm. Layer-by-layer growth could be achieved for film thicknesses up to 400 nm as monitored by reflection high-energy electron diffraction and confirmed by X-ray diffraction. We obtained a constant microwave resistivity of 29 $\mu\Omega$cm between 0.1 and 20 GHz by refining the frequency dependence of the transmission coefficients. Our result shows that $SrMoO_3$ is a viable candidate as a highly conducting electrode material for all-oxide microwave electronic devices. This work was supported by the DFG project KO 4093/1-1.

[1] A. Radetinac, A. Mani, S. Melnyk, M. Nikfalazar, J. Ziegler, Y. Zheng, R. Jakoby, L. Alff, and P. Komissinskiy, Appl. Phys. Lett. **105**, 114108 (2014)

Topical Talk MM 46.8 Thu 12:30 EB 407

Tunable GHz-components with ferroelectric and liquid crystal technologies for mobile terrestrial and satellite-based systems — •Rolf Jakoby — Institute of Microwave Engineering and

Photonics, Technische Universität Darmstadt, Merckstr. 25, 64283 Darmstadt, Germany

Recent progress in Liquid Crystal (LC) technology made in Darmstadt is very promising for next-generation reconfigurable/tunable microwave and millimeter wave devices because they exhibit excellent properties at high frequencies above 15 GHz, since LC losses generally decrease with increasing frequency. This opens up new low-cost LC applications beyond optics. In contrast, ferroelectric material, particularly Barium Strontium Titanate (BST), is well suited at frequencies below 15 GHz, using screen and inkjet printing of BST layers. Hence, with these two material classes, we can cover a frequency range from 1 GHz up to 1 THz for tunable components such as varactors, tunable delay and loaded lines, phase shifters, tunable filters, adaptive matching networks, tunable frequency selective surfaces, tunable multiband antennas, polarization-agile antennas, phased-scanning reflect- and phased arrays. This contribution presents an overview of the both technologies, BST and LC, including basic principles, tuning mechanisms, processing technologies, device concepts and design, packaging and integration issues as well as functional tests with focus on frequency-agile multiband antennas and filters as well as electronically beam-steering antennas for mobile terrestrial and satellite-based applications.

MM 47: Invited talk Korte

Time: Thursday 9:30–10:00 Location: TC 006

Invited Talk MM 47.1 Thu 9:30 TC 006

Small experiments but great insights * Plasticity in brittle materials — •Sandra Korte-Kerzel, Harshal Mathur, and Sebastian Schröders — Institut für Metallkunde und Metallphysik, RWTH Aachen University, Germany

Hard and brittle materials are used in many modern applications, from semiconductors over wear-resistant coatings to high temperature materials. Although most of their properties are well known, very little is often understood with regards to their plastic deformation. However, failure can frequently occur by just that and the use of promising high temperature materials is often hampered by low temperature brittleness, where a better understanding of the underlying deformation mechanisms could support new alloying strategies. The reason for this gap in our understanding is due to the experimental difficulties normally encountered in studying plasticity in brittle materials. Due to catastrophic failure during testing, subsequent analysis of deformation mechanisms is impeded and suppression of cracking can conventionally only be achieved by means of confining pressure. Recently, it has been shown that microcompression can help overcome these challenges and therefore plasticity of brittle materials can now be studied relatively easily and in near uniaxial stress-states. By extending this technique to elevated temperatures, deformation mechanisms based on thermal activation of dislocation glide in hard materials become accessible and studies on small single crystalline specimens can shed light on many questions regarding deformation, including plastic anisotropy and the activation of individual slip systems.

MM 48: Methods in Computational Materials Modelling VI: Algorithms

Time: Thursday 10:15–11:30 Location: H 0106

MM 48.1 Thu 10:15 H 0106

Molecular-Dynamics Simulations on Many-Core Processors — •Ralf Meyer and Chris Mangiardi — Laurentian University, Sudbury, Canada

Molecular-dynamics (MD) simulation is one of the most important methods for the numerical studying of materials. This contribution discusses new algorithms for large-scale MD simulations on modern CPUs. Forthcoming many-core processors will soon integrate hundreds of compute cores in a single processor with SIMD units that operate on vectors of 8 or more double-precision numbers simultaneously. However, the full power of these devices will only be accessible with the help of novel algorithms.

The cell task method [1,2] uses a task-based programming approach for the parallelization of MD simulations on multi- and many-core architectures. The method avoids load balancing problems by using a large number of dynamically scheduled small tasks to distribute the workload among the processing cores. Furthermore, a tiling algorithm is used that increases the efficiency of wide SIMD vector units in the simulations.

Results from benchmark simulations on Xeon Phi co-processors are presented. The results show that the cell task algorithm scales well for large numbers of threads. In addition to this, the method outperforms the spatial decomposition approach for simulations of inhomogeneous (e.g. porous) systems.

[1] R. Meyer, Phys. Rev. E **88**, 053309 (2013).
[2] R. Meyer, J. Phys.: Conf. Ser. **540**, 012006 (2014).

MM 48.2 Thu 10:30 H 0106

Studies of thermomechanical properties and nanoscale phase transitions using the universal multiscale computer program MBN Explorer — •Christian Kexel[1,2] and Andrey Solov'yov[1,2] — [1]Department of Physics, Goethe University, 60438 Frankfurt, Germany — [2]MBN Research Center, 60438 Frankfurt, Germany

We present the popular multipurpose computer code MBN Explorer (MesoBioNano Explorer) which allows modeling molecular systems of varied level of complexity. The package is suited to compute system's energy, to optimize molecular structures as well as to simulate many molecular systems with sizes ranging from the atomic to the mesoscopic scales by means of molecular-dynamics and kinetic monte-carlo approach. A distinct feature of the program, which makes it significantly different from existing codes, is its universality and applicability to the description of a broad range of problems comprising atomic clusters, nanotubes, fullerenes, polypeptides, proteins, DNA, composite systems and nanofractals. In particular, we present our research on the thermomechanical properties of various materials and the study of nanoscale phase transitions.

MM 48.3 Thu 10:45 H 0106

A QM/MM method to study solid-solid interfaces — •Sara Panahian Jand[1], Pouya Partovi-Azar[2], Setareh Javadi Dogahe[1], and Payam Kaghazchi[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Department Chemie, Technische Chemie, Universität Paderborn, 33098 Paderborn, Germany

The hybrid quantum mechanics/molecular mechanics (QM/MM) approach is a promising method to study large systems on the atomic scale. In this work we present our recently developed QM/MM method that can be used to study solid-solid interfaces. In this method, the QM region is described by density functional theory (DFT). For the MM region we discuss the influence of choosing different classical potentials on the QM/MM results. The point charges which are required for the coulomb interactions as well as van der Waals parameters are obtained independently by fitting the classical potentials to DFT-based electrostatic energies and long-range dispersion energies (calculated by the Quantum Harmonic Oscillator model with Maximally Localized Wannier Functions), respectively. The remaining parameters for the MM region are evaluated by comparing physical quantities calculated with DFT and those calculated with classical potentials. We finally show the application of our QM/MM approach to study solid electrolyte interphases in Li-ion batteries.

MM 48.4 Thu 11:00 H 0106

Ab-initio non-linear optics beyond the long-wavelength limit. — •Klaus-Dieter Bauer, Martin Panholzer, and Kurt Hingerl — Johannes Kepler Universität, Linz, Österreich

In ab-initio methods optical properties are typically evaluated in the long-wavelength limit, which leads to questionable results for absorbing systems in general and specifically predicts zero bulk contribution to second harmonic generation, while experimental results show a bulk contribution from small-wavelength components of the field.

We try to establish how these effects are related to the full microscopic second-order response function $\chi^{(2)}(\mathbf{k}_0, \omega_0; \mathbf{k}_1, \omega_1, \mathbf{k}_2, \omega_2)$ and how to obtain effective local response functions from DFT.

MM 48.5 Thu 11:15 H 0106

Test set for materials science and engineering — Toktam Morshedloo[1,2], •Norina A. Richter[1], Fawzi R. Mohamed[1], Xinguo Ren[3], Sergey V. Levchenko[1], Luca M. Ghiringhelli[1], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Ferdowsi University of Mashhad, Mashhad, IR — [3]University of Science and Technology of China, China

Understanding of the applicability and limitations of electronic-structure methods needs detailed comparison with highly accurate data of representative test sets. A variety of highly valuable test sets have been established in quantum chemistry for small molecules. However, for crystalline solids they are still lacking. We present a representative test set for materials science and engineering (MSE) which includes first and second row elements and their binaries, comprising various crystal structures. This allows for unbiased benchmarking for various chemical interactions. In the MSE test set, we consider cohesive energy, lattice constant, bulk modulus, electronic band structures, and phonons etc. A big effort is made to produce systematically converged results with respect to basis set[1] and **k** mesh for a hierarchy of electronic-structure methods, ranging from the local-density approximation to advanced orbital-dependent functionals implemented in the all-electron, full-potential FHI-aims code. Furthermore, we use incremental schemes to obtain benchmark values calculated with coupled-cluster approaches. [1] I. Y. Zhang *et al.*, *NJP* **15** 123033 (2013)

MM 49: Interfaces I: Structure and Segregation

Time: Thursday 10:15–11:45 Location: H 0107

MM 49.1 Thu 10:15 H 0107

First-principles and tight-binding studies of symmetrical tilt grain boundaries in bcc-Fe — •Jingliang Wang, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universitätsstr. 150, D- 44801 Bochum, Germany

Using density functional theory (DFT), we studied the stability of a series of low-Σ symmetrical tilt grain boundaries (STGBs) in bcc-Fe. A systematic strategy was applied to seek the most stable configuration. All STGBs studied in this work possess a similar GB energy except for the more stable Σ3(112)-GB. We present the correlations between the GB energies and local atomic structures. Based on the results from DFT calculations, we modified the recently-developed othogonal tight-binding (TB) model for iron and we show that the modified TB model is able to predict the correct GB structure and give GB energies in good agreement with DFT. We validated the model for twist GBs and apply it to study the stability of realistic models of GBs in martenstic steels.

MM 49.2 Thu 10:30 H 0107

On the origin of anisotropic lithiation of Si — •Ashkan Moradabadi[1], Jochen Rohrer[2], Karsten Albe[2], and Payam Kaghazchi[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustrasse 3, 14195 Berlin, Germany — [2]Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Si nanowires (SiNW) are promising candidates for next-generation lithium-ion battery anodes. Lithiation of SiNW anodes proceeds by the movement of interfaces between lithiated amorphous Li_xSi and pristine crystalline Si in a core-shell structure. Experimental studies show that first-cycles of lithiation of SiNWs lead to an anisotropic expansion of SiNWs. In this work, we present density functional theory calculations on Li incorporation in SiNWs using surface and interface geometries. We find that in opposition to the results based on (commonly-used) surface models, the anisotropic expansion of SiNWs does not originate from orientation-dependent barriers for Li diffusion across the Li_xSi/Si interfaces. Due to the disorder nature of interfaces these barriers are distributed isotropically. Instead, here we find that the anisotropic swelling is a consequence of orientation-dependent interface energies and the fact that high-energy interfaces are more mobile than low-energy interfaces.

MM 49.3 Thu 10:45 H 0107

Why calculated energies of grain boundary segregation are unreliable when segregant solubility is low — Pavel Lejček[1], •Mojmír Šob[2,3,4], Václav Paidar[1], and Václav Vitek[5] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [5]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA

We demonstrate that density functional theory based calculations of segregation energies at interfaces are often unreliable when the bulk solid solubility of the segregant is lower than that corresponding to one solute atom per computational repeat cell. In this case, the calculated energy of a solute in the bulk cannot be used when evaluating segregation energies. We document this problem by analyzing the measured and calculated grain boundary segregation energies in nickel and bcc iron available in the literature. On the other hand, even when using repeat cells that are not sufficient for reliable evaluation of the segregation energy, the change in the grain boundary cohesion (strengthening/embrittling energy) may be obtained with a reasonable accuracy.

MM 49.4 Thu 11:00 H 0107

Tensile strength of Ni grain-boundary with segregated sp-impurities — •Miroslav Černý[1,2,3], Petr Šesták[1,2], Petr Řehák[1,2,3], Monika Všianská[1,3], and Mojmír Šob[1,3,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic — [4]Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GB) represent extended planar defects with a crucial effect on macroscopic strength of polycrystalline materials. In this first principles study, we calculate the ideal tensile strength of Σ5(210) tilt GB in nickel crystal under uniaxial loading applied perpendicularly to the GB plane. A repeat cell containing 64 atoms is subjected to three different modes of simulated deformation comprising rigid grain shift, uniaxial deformation with optimized atomic coordinates and fully optimized uniaxial loading (ionic positions in the supercell as well as the cell shape are optimized at each step of deformation). Results for these models are compared and tensile strength of clean GB is compared with that of GB with segregated impurities (S and Al) and with the results of previous studies. Differences in computed values show not only the effect of the impurities on the ideal strength but also the importance of full lattice optimization during the simulation of tensile test.

MM 49.5 Thu 11:15 H 0107

Theoretical strength of Σ5 (210) GB in FCC cobalt with segregated interstitial and substitutional sp-impurities — •Petr Šesták[1,2], Miroslav Černý[1,2,3], Petr Řehák[1,2,3], Monika Všianská[1,3], and Mojmír Šob[1,3,4] — [1])Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic — [4]Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GBs) determine many mechanical properties of polycrystalline materials, in particular their strength. Moreover, the impurities contained in the material tend usually to segregate at the

GBs and thus they can have a strong negative or positive influence on its mechanical characteristics. In this first-principles study we simulate the uniaxial tensile test of FCC cobalt containing the Σ5 (210) tilt GB with segregated sp-impurities. The uniaxial deformation was performed along an axis perpendicular to the GB. The impurities Al, Ga, In, Sn, Sb and Te were considered in substitutional positions at the GB and Si, P, S, Ge, As and Se in interstitial positions. The strength of segregated GBs was compared with the strength of the clean GB. The uniaxial deformation was realized using two different approaches. In the first one the repeat cell was continually optimized during the entire deformation path and in the second one the deformation corresponded to a rigid separation of grains along a defined plane without any cell optimization.

15 min. break

MM 50: Biomaterials and Biological Materials III

Time: Thursday 10:15–11:45 Location: TC 006

Topical Talk MM 50.1 Thu 10:15 TC 006

Entwicklung von bioresorbierbaren Magnesiumimplantaten für individuelle Kontinuitätsdefekte in der MKG-Chirurgie — •Ralf Smeets[1], Ole Jung[1], Henning Hanken[1], Max Heiland[1], Christoph Ptock[2], Max Schwade[3], Alexander Kopp[2] und Philip Hartjen[1] — [1]Klinik und Poliklinik für Mund-, Kiefer- und Gesichtschirurgie, Universitätsklinikum — [2]Meotec GmbH & Co. KG — [3]Werkzeugmaschinenlabor WZL der RWTH Aachen

Großvolumige Knochendefekte nach Trauma- oder Tumorresektionen im Gesichtsbereich erfordern den Einsatz von Knochentransplantaten oder rekonstruktiven Materialien wie Titan. Herkömmliche Verfahren ziehen oft erneute operative Eingriffe mit entsprechenden Morbiditäten und möglichen Komplikationen für den Patienten nach sich. Das Projekt BIOMAGIK verfolgt die Entwicklung von Implantaten aus Magnesium, die durch ihre vollständige Degradierbarkeit und knochenähnlichen Eigenschaften die bestehenden Probleme lösen sollen. Die Implantate werden durch funkenerosive Bearbeitung maßgeschneidert und mit einer osseoinduktiven Makrostruktur versehen. Das Degradationsprofil wird durch Konversion der Oberfläche in eine resorbierbare Keramik optimiert. Hier zeigen wir die Charakterisierung der Implantatmaterialien hinsichtlich Degradationskinetik, in vitro Biokompatibilität und Oberflächeneigenschaften.

MM 50.2 Thu 10:45 TC 006

Response of rat bone structure and mineralization to a degrading Magnesium implant — Tilman Grünewald[1], Harald Rennhofer[1], Martin Meischel[1], Vicki Nue[2], Bernhard Hesse[3], Manfred Burghammer[3], Alessandra Gianoncelli[4], Henrik Birkedal[2], Marine Cotte[3], Annelie Weinberg[5], Stefanie Stanzl-Tschegg[1], and •Helga Lichtenegger[1] — [1]Inst. of Physics and Materials Science, Univ Natural Resources and Life Sciences, Vienna, Austria — [2]iNANO, University of Aarhus, Denmark — [3]ESRF, Grenoble, France — [4]Elettra Sincrotrone, Trieste, Italy — [5]Dept. Orthopedics & Orthopedic Surgery, Med Univ Graz, Austria

Biodegradable bone implant materials are of special interest for medical application specifically in children, where traditional implants have to be removed in a second surgery in order not to disrupt bone growth. In this study we investigated the response of bone mineralization to a degradable Mg implant in a rat model (Sprague-Dawley rat) over a growth period from 1-18 months. Alterations in the bone nano- and mineral structure were investigated by synchrotron-based methods such as small-angle x-ray scattering (SAXS) and diffraction (XRD), x-ray fluorescence (XRF), as well as x-ray absorption spectroscopy (XAS) at a spatial resolution of about 3 micrometer. The combined study showed nanostructural changes at the interface to the degrading implant, but also changes in the bone mineral structure by the presence of Mg ions. Interestingly Mg enrichment was also found around blood vessels several hundreds of micrometer away from the bone-implant interface, which sheds light on possible Mg transport mechanisms.

Topical Talk MM 50.3 Thu 11:00 TC 006

3D scaffolds as cell adhesion templates — •Christine Selhuber-Unkel — Biocompatible Nanomaterials, Institute of Materials Science, University of Kiel, Kiel, Germany

3D biomaterial scaffolds are promising materials for mimicking the natural environment of many cell types. In particular, materials with high structural flexibility offer interesting possibilities, e.g. for mimicking extracellular matrix in order to achieve directed cell growth. We have developed methods to generate 3D biomaterials that contain interconnected structural micro- and nanoelements. In addition to controlling scaffold structure and porosity, we can also define scaffold stiffness, conductivity and surface functionalization. Intriguingly, cells can grow deeply into such scaffold materials and the scaffolds can induce cell functionalities, thus possibly leading to future tissue engineering applications.

15 min. break

MM 51: Mechanical properties II

Time: Thursday 10:15–11:45 Location: TC 010

MM 51.1 Thu 10:15 TC 010

Velocity strengthening friction significantly affects interfacial dynamics, strength and dissipation — •Robert Spatschek[1], Marc Weikamp[1], Efim Brener[2], Yohai Bar-Sinai[3], and Eran Bouchbinder[3] — [1]Max-Planck Institut für Eisenforschung, Düsseldorf — [2]Peter-Grünberg-Institut, Forschungszentrum Jülich — [3]Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel

Frictional processes are a natural feature of our daily life, yet their dynamics are not well understood. Recent experimental data have revealed that velocity strengthening friction, where frictional resistance increases with sliding velocity over some range, is a generic feature of such interfaces. Moreover, transitions between velocity weakening and strengthening regimes have recently been linked to slow fronts ("slow earthquakes"). Here we elucidate the importance of velocity strengthening friction by theoretically studying variants of a realistic friction model, all featuring identical logarithmic velocity weakening at small sliding velocities, but different high velocity behaviour. We find a dramatic influence on front velocity, event magnitude, dissipation and radiation rates. Additionally, we show that velocity strengthening can give rise to a new kind of frictional instability for sliding on a rigid substrate, which is related to interval vibrational high frequency excitations in the sliding object.

MM 51.2 Thu 10:30 TC 010

microstructure evolution of brass alloys under dry reciprocating tribological loading — •zhilong liu[1], philipp messer[1], peter gumbsch[1,2], and christian greiner[1] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, Kaiserstrasse 12, 76131 Karlsruhe, Germany — [2]Fraunhofer IWM, Woehlerstrasse 11, 79108 Freiburg, Germany

Correlating a material's microstructure with its friction and wear properties is a central question in tribology. Still, there are many open questions concerning the mechanistic understanding of the microstructure evolution under a tribological load.

Different brass alloys with zinc contents between five and 36% in contact with silicon nitride were used as model tribosystems. Between these alloys, the stacking fault energy varied by more than a factor of five. Starting with an annealed microstructure, we systematically varied the sliding distance and followed the evolution of the microstructure by scanning electron and focused ion beam microscopy. A tribo-

logically deformed layer was observed after the tests, whose thickness increased with the sliding distance. Comparing the results for different brass alloys and those for high-purity copper, an effect of increasing zinc content was observed.

A long term goal of this study is to formulate a mechanistic model description for the microstructural changes in tribological contacts, including the influence of different stacking fault energies in face-centered cubic metals. This might allow for materials with tailored microstructures combing low friction forces and small wear rates.

MM 51.3 Thu 10:45 TC 010

Nanotribology induced Microstructure Evolution in Pearlite — •Caroline Fink, Steffen Brinckmann, Sunmi Shin, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Tribology has long been understood as a hierachical phenomenon: nanoscale asperities exist on mesoscale asperities which exist on macroscopic asperities. Hence, tribology is a multiscale mechanism that spans multiple orders of length scales. We focus on tribological experiments at the micro- and nanoscale in iron alloy micro-structures to fundamentally understand tribology. The aim of this study is to upscale these findings to the friction and wear behavior at the macroscale. We prepare pearlite samples with varying carbon content and highlight the preparation requirements for experiments at the nanoscale. Single stroke scratches are performed and used to provide microstructure specific friction coefficients and scratch depths. Post-deformation investigations by atomic force microscopy, scanning electron microscopy and confocal microscopy reveal the microstructure dependent pile-up and real contact area. Cross-sections by focused ion beam milling show the nanotribology induced sub-surface microstructure which we relate to the cemetite lamellae orientation and spacing. Finally, we will highlight the influence of the nanoscale counter-body shape on the wear resistance and the friction coefficient.

MM 51.4 Thu 11:00 TC 010

Roughness and Microstructure Development during Nanotribology in Austenite — •Steffen Brinckmann, Caroline Fink, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Materials wear is the collective contact on a number of hierarchical length scales. The macroscopic surface has microscopic surface roughness which itself has an almost atomistic surface roughness superimposed. We study wear at the microscopic lengthscale by using a single hard asperity and study the deformation of the flat Austenite steel. Single stroke experiments reveal that the plasticity and roughness are determined by the local grain orientation. Moreover, the symmetric scratch loading can lead to unsymmetrical slip patterns, when comparing both sides of the scratch. We find that analytical equations based on the Hertz solution and the Hardness equation predict the elastic and plastic scratch depth for multiple orders of normal force, although both equations were developed for the static indentation loading and not the present dynamic scratch loading. Finally, we will discuss the formation of cracks and surface roughness in the scratch tracks. We close with a discussion on the addition of the plasticity induced surface roughness to the hierarchical length scales in tribology.

MM 51.5 Thu 11:15 TC 010

Investigation of VHCF behavior of an austenitic-ferritic duplex steel during insitu XRD measurements with different load amplitudes — •Anne K. Hüsecken[1], Marcus Söker[2], Ulrich Krupp[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Siegen, Germany — [2]Hochschule Osnabrück, Osnabrück, Germany

The behavior of materials in the region of very high cycle fatigue (VHCF) is not known, yet. Nowadays, with the development of ultrasonic testing machines (BOKU Vienna), it is possible to reach the region over 10 million cycles within a few hours. One of these machines was directly mounted on the diffractometer at beamline BL 10 at DELTA in Dortmund, to investigate the behavior of single grains within the flat dogbone-shaped austenitic-ferritic duplex steel samples (1.4462) during the whole fatigue process of the sample. Therefore Rockingscans were performed after each fatigue step with different load amplitudes, analyse FWHM and peak positions. In former studies we already showed, that it is possible to analyse one single grain by this method [1]. We found, that some grains rotate or change their lattice orientations during fatigue [2]. The analysis and results of these XRD measurements will be presented.

[1] K.Istomin et al., Int. J. of Fatigue 66 (2014), 177-182.
[2] A.K. Hüsecken et al., Procedia Engineering 74 (2014), 53-56.

15 min. break

MM 52: Nanomaterials III: Nanoporous Gold and Phase Transformations

Time: Thursday 11:45–13:15 Location: H 0106

MM 52.1 Thu 11:45 H 0106

***In situ* mechanical testing of nanoporous gold: new insights into plasticity of nanostructures** — •Nadiia Mameka[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht — [2]Technische Universität Hamburg-Harburg

Surface plays a significant role in plasticity of nanoscale objects. This has been well documented by the size-dependent strength in recent studies on nanowires. Our research aims to contribute towards identifying the underlying processes for the observation by employing nanoporous gold (np-Au), as a material with large specific surface area in a network of nanowires or nanoligaments. The millimeter-seized np-Au samples were tested *in situ* in compression under potentiostatic control in aqueous electrolytes. The amount of the surface area was tuned by structural coarsening, while the state of the surface was controlled by application of an electrical potential E.

The electrode polarization of the Au-electrolyte interface results in an effective strengthening of np-Au by negative charging and specific adsorption at the surface. The overall flow stress σ_F as well as its potential-induced changes $\Delta\sigma_F/\Delta E$ scale with the ligament size. Remarkably, when normalized by the actual stress, the flow stress-potential coupling parameter $\Delta\sigma_F/\Delta E$ exhibits no size-dependence. This finding implies an important link between phenomena responsible for strengthening by electric potentials and strengthening by structural size. In this respect possible relevant mechanisms that control the plastic deformation will be discussed.

MM 52.2 Thu 12:00 H 0106

Investigation of the Deformation Behavior of Nanoporous Metals Using Digital Image Correlation — •Lukas Lührs[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg — [2]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht

Nanoporous metals have an extremely high specific surface area. This makes them of interest for studies of small-scale deformation, since the mechanical behavior can be manipulated through number and properties of the surfaces. A fundamental issue in elastic as well as plastic deformation of nanoporous metals is the transverse coupling, in other words, the link between longitudinal and transverse strain under uniaxial loading conditions. Millimeter sized nanoporous gold samples with different ligament size were prepared via dealloying and tested mechanically under single and cyclic compression up to strains of 50%. By using a digital image correlation set-up, 2-dimensionally resolved strain measurements of the sample surface could be obtained, enabled by full field displacement calculations upon loading. Among other material properties, the development of the elastic and plastic Poisson's ratio during the deformation process was determined. In each instance the lateral deformation is small. Yet, the transverse coupling does not vanish; this is contrary to some previously published claims. Furthermore, a significant dependence of the Poisson's ratio on the ligament size as well as the macroscopic strain was observed.

MM 52.3 Thu 12:15 H 0106

Investigation of the coarsening behaviour of nanoporous gold based on representative volumes — Kaixiong Hu[1], •Markus Ziehmer[1], Ke Wang[2], and Erica Lilleodden[1] — [1]Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Geesthacht, Germany — [2]Hamburg University of Technology,

Institute of Materials Physics and Technology, Hamburg, Germany

Advances in 3D analyses by electron microscopy enable the detailed investigation of material systems exhibiting complex microstructures, such as nanoporous gold (npg). This in turn allows access to critical structural parameters needed to advance our understanding of material behaviour. In particular, the coarsening of the 3D bicontinuous pore-ligament network of npg is one problem, where 3D analysis helps to explore the applicability of scaling laws in mechanical behaviour, which implicitly assume structural self-similarity across varying length-scales. However, reliable answers require a careful identification of representative volumes, which mimic the characteristics of the global microstructure. We present an investigation on thermally induced coarsening of npg based on focused ion beam tomography. The presentation highlights the importance of properly identifying representative volumes for this type of material system. Results on crucial microstructure parameters like ligament size, surface curvature and network connectivity are shown, which seem to support the view of structural self-similar evolution of npg.

MM 52.4 Thu 12:30 H 0106

Influence of elastic stresses during the formation of hollow nanoparticles — •Manuel Roussel and Guido Schmitz — Lehrstuhl für Materialphysik, Universität Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany

The formation of hollow particles has been extensively studied during the past few years, and this enthusiasm assuredly comes from the fact that nanometric containers may have several applications in various fields (drug delivery, catalysis, composite materials). A multitude of various hollow architectures have been created, using various methods, as reported in hundreds of publications. However, numerous fundamental questions have not been clarified yet.

This project aims at investigating one of these questions. What mechanisms are involved during the creation of a hollow particle at the atomic scale? More precisely, we try to understand the link between solid state diffusion, non-equilibrium vacancies and diffusion-induced stresses during the formation of a Kirkendall void in core-shell nanostructures.

While finite element simulations allow us to apprehend the problem from a theoretical point of view, we also have a powerful characterization tool at our disposal: the Tomographic Atom Probe (TAP). Here, emphasis will be placed on showing how diffusion and phase transformation can be controlled using stress and geometry in a nanostructure. For instance, we will show how switching from a nanosphere to a nanowire configuration can drastically change diffusion kinetics at the atomic scale.

MM 52.5 Thu 12:45 H 0106

Molecular-dynamics simulation of martensite-austenite transition in nickel-titanium nanoparticles — •Christian Kexel[1], Stefan Schramm[1,2], and Andrey Solov'yov[1,3] — [1]Department of Physics, Goethe University, 60438 Frankfurt, Germany — [2]Frankfurt Institute for Advanced Studies, Goethe University, 60438 Frankfurt, Germany — [3]MBN Research Center, 60438 Frankfurt, Germany

Shape-memory alloys can after initial deformation reconstruct their pristine structure upon heating. The underlying phenomenon is the structural solid-solid transformation from low-temperature lower-symmetry martensite to high-temperature higher-symmetry austenite. The near-equiatomic NiTi possesses an eminent importance for biomedical applications whereas the nanostructured equivalent can exhibit yet enhanced thermomechanical properties. However, no plausible microscopic theory of the shape-memory effect in NiTi exists, especially for the nanoscale systems. In this work, the thermally-induced martensite-austenite transition in free nanocrystals with 8472 to 39349 atoms is investigated by means of classical molecular-dynamics simulations. Thereby a recently published study is complemented. Interatomic interactions are modeled by a semi-empirical many-body potential based on tight-binding second-moment approximation. The structural transition, revealing features of a first-order transformation, is successfully demonstrated and contrasted with melting, a quantum harmonic model and experimental findings. Moreover, a nucleation-growth process is observed as well as the irreversibility of the transition.

MM 52.6 Thu 13:00 H 0106

MORPHOLOGY AND PHASE TRANSFORMATION OF INDIUM NANOPARTICLES EMBEDDED IN AN ALUMINUM MATRIX — •Mostafa Mohamed, Martin Peterlecher, and Gerhard Wilde — Institute of Materials Physics, Münster, Germany

The melting , undercooling, and superheating of In- nanoparticles embedded in an Al matrix have been studied as a function of particle size by differential scanning calorimetry (DSC) and transmission electron microscopy (TEM). Different densities of nanometer-sized In particles that were uniformly embedded in an Al-matrix have been synthesized by rapid melt quenching. After systematic thermal treatments, a portion of the In-particles showed an increase of the melting temperature compared to the bulk behavior. Analyses of DSC measurements and TEM images were carried out to analyze the impact of the interfaces between nanoparticles and matrix as well as of pressure effects on the melting/freezing phase transformation. The properties of embedded and grain boundary particles are also discussed.

MM 53: Interfaces II: Deformation and Motion

Time: Thursday 11:45–12:30 Location: H 0107

MM 53.1 Thu 11:45 H 0107

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

A comparison of microstructures and properties in materials subjected to the later stages of severe plastic deformation (SPD) or steady-state superplastic flow indicates several unexpected similarities especially with respect to the interface response on the deformation, such as grain boundary (GB) sliding events, which lead to a suppression of dislocation activity. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle GBs in SPD-processed materials in terms of the concept of shear localization in the interfaces. For this purpose, oblate spheroids of a few atomic diameters size have been chosen as the basic units of sliding. By performing atomistic simulations of these special grain boundaries, their response to deformation is analysed. Different properties, as e.g. the coupling of grain boundary motion in normal direction to a shear deformation parallel to the grain boundary or the grain boundary stiffness and the local shear modulus are calculated and compared to those of relaxed high angle grain boundaries.

MM 53.2 Thu 12:00 H 0107

Shearing behaviour of interfaces: linking intrinsic properties with deformation mechanisms — Mansour Kanani, Alexander Hartmaier, and •Rebecca Janisch — ICAMS, Ruhr Universität Bochum, 44780 Bochum

In many interface-dominated nanostructured materials the role of interfaces during deformation is not yet completely clarified. Very fine spacing of interfaces leads to a competition between dislocation controlled and grain boundary sliding based plasticity. To improve our understanding of this competition we have to investigate the atomistic origin of ductility in the interface region. A multi-scale concept is introduced to capture effects of both the electronic and the atomistic level at interfaces in nano-lamellar TiAl alloys. First, we carried out quasi-static calculations of multi-planar generalized stacking fault energy (M-γ) surfaces of the interface plane as well as the adjacent layers. Second, molecular dynamics simulations guided by ab initio γ-surface calculations were carried out for different bicrystal cells under different shear loading conditions. The results show various shear mechanisms such as twin nucleation and migration/absorption, interface partial dislocation nucleation, and rigid grain boundary sliding/migration. The comparison with the M-γ-surfaces allows to create a link between physical properties and deformation mechanisms, and hence between the results of ab-initio calculations and molecular dynamics simulations. Furthermore we discuss the interplay between interface geometry, atomistic structure, and loading conditions, and its impact on the

deformability of lamellar microstructures.

MM 53.3 Thu 12:15 H 0107

Molecular dynamics study of the migration kinetics of asymmetric grain boundaries — •Sherri Hadian[1], Blazej Grabowski[1], Christopher Race[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisen Forschung,max planck str 1,Düsseldorf,40237 — [2]The university of Manchester, Manchester, UK

Classical molecular dynamics (MD) simulations are commonly used to explore the migration of grain boundaries. Our previous research on low sigma symmetric boundaries has shown that at conditions of low driving forces as found in actual experimental setups and when going towards system sizes exceeding those commonly employed in MD a novel mechanism becomes operational that is based on mesoscopic island nucleation. [1] In the present study we extend our research towards grain boundaries deviating from the perfect and symmetric arrangement to investigate the kinetics of asymmetric, defective boundaries. Such grain boundaries constitute in fact the majority of experimentally observed moving boundaries. We introduce defects by deviating the boundary plane from a symmetric equilibrium boundary. The results of the simulations show how the fundamental atomistic mechanisms change as the nucleation driven motion shifts towards a step propagating one. [1] - C. P. Race, J. von Pezold, and J. Neugebauer. Phys. Rev. B 89, 214110.

MM 54: Biomaterials and Biological Materials IV

Time: Thursday 11:45–13:00 Location: TC 006

MM 54.1 Thu 11:45 TC 006

Hierarchical macroscopic fibrillar adhesives: In situ study of buckling and adhesion mechanisms on flat and wavy surfaces — •Christina Bauer[1,2], Elmar Kroner[1], Norman Fleck[3], and Eduard Arzt[1,2] — [1]INM - Leibniz Institute for New Materials, Campus D2 2, Saarbruecken, Germany — [2]Saarland University, Campus D2 2, Saarbruecken, Germany — [3]Cambridge University Engineering Department, Trumpington Street, Cambridge, CB2 1PZ, UK

Nature uses hierarchical fibril structures to adhere temporary to any kind of surfaces. To understand the effect of hierarchy, the adhesion and buckling of macropatterned adhesives in contact with flat and wavy surfaces was investigated. Macroscopic models possessing up to three hierarchy levels in the range of 0.3 to 4.8 mm were fabricated from polydimethylsiloxane by a soft molding process. For both flat-ended and mushroom-shaped samples, experimental and theoretical studies indicate that the buckling load for hierarchical structures is 4-5 times less than that needed to induce buckling in the single-level structures due to a change in the buckling mode. Such buckling events lead to a loss in surface contact, which diminishes adhesion. Consequently, the number of hierarchy levels was found to strongly influence adhesion.

MM 54.2 Thu 12:00 TC 006

Understanding Macroscopic Interfacial interactions based on Single Molecule Energy Landscapes — Sangitha Raman, Thomas Utzig, Philipp Stock, and •Markus Valtiner — Max-Planck-Institut für Eisenforschung GmbH, Department for Interface Chemistry and Surface Engineering,D-40213 Düsseldorf, Germany

Understanding cell adhesion on metals and oxides, cell-cell interaction or interfaces in biomaterials based on single molecular level details relies on understanding the scaling of single molecule interactions towards integral interactions at the meso- and macroscopic scale. Here, we discuss how one can decipher the scaling of individual single acid-amine interactions towards the macroscopic level, where a large number of these bonds interacts simultaneously, using a synergistic experimental approach combining Surface Forces Apparatus (SFA) experiments and single molecule force spectroscopy (SMFS). We show that equilibrium SFA measurements scale linearly with the number density of acid-base bonds at an interface, providing acid-amine interaction energies of $10.9 \pm 0.2\,kT$. SMFS similarly converges to an interaction energy of $11 \pm 1\,kT$, with unbinding energy barriers of $25\,kT \pm 5\,kT$. Finally, we will also show how other specific adhesive bonds such as the Amine/Gold binding can be successfully studied in the contest of our approach. As such, our experimental strategy provides a unique framework for molecular design of novel functional materials through predicting of large-scale properties such as adhesion, self-assembly or cell-substrate interactions based on single molecule energy landscapes.

MM 54.3 Thu 12:15 TC 006

The influence of reversible cross-links on the mechanical properties of chain-bundle systems — •S. Soran Nabavi and Markus A. Hartmann — Institute of Physics, Montanuniversität Leoben, Leoben, Austria

Although biological materials use a very limited number of base elements to build their structures, these structures show an enormous diversity of mechanical properties. One effective strategy to increase the toughness of these materials is using reversible cross-links in their structures. These so called sacrificial bonds can be found in a large variety of biological materials e.g. bone, wood and in softer fibers like silk and byssal threads. We use Monte Caro simulations to examine the influence of grafting density and cross-link density on the mechanical properties of the chain bundle by determining load-displacement curves. Most surprisingly the results show that only two cross-links are sufficient to break the backbone of the system although the cross-links are weaker than the covalent bond by factor of four. This failure is caused by the topology of the interchain cross-links in the chain bundle where sacrificial bonds are distributed in an ordered arrangement. This backbone failure weakens the strength of the material, but increases the amount of work to elongate the system as well as the apparent stiffness of the bundles. These results bear important implications for the understanding of natural systems and for the generation of strong and ductile biomimetic polymers.

MM 54.4 Thu 12:30 TC 006

Quantum-mechanical study of isotropic elastic properties of amorphous $CaCO_3$ — •Martin Friák[1,2], Gernot Pfanner[2], David Holec[3], Biyao Wu[2,4], Helge Otto Fabritius[2], Dierk Raabe[2], and Jörg Neugebauer[2] — [1]Institute of Physics of Materials AS CR, v.v.i. Brno, Czech Republic — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Montanuniversität Leoben, Leoben, Austria — [4]RWTH Aachen University, Aachen, Germany

Nearly 80 % of all known animal species are protected by an exoskeleton formed by their cuticle. The cuticle represents a hierarchically structured multifunctional bio-composite based on chitin and proteins. Some groups like Crustacea reinforce the load-bearing parts of their cuticle with amorphous $CaCO_3$ (ACC) in the form of nano-scopic particles. As these particles are too small to be probed experimentally, we use quantum-mechanical methods to determine the phase stability and elastic properties of ACC employing a supercell approach. Our study is focused on the identification of a suitable computational supercell to be used as a structural model for ACC. Amorphous $CaCO_3$ lacks any periodic structural order and it is thus perfectly incompatible with the concept of computational supercells that are periodically repeated by inherent boundary conditions applied in most of computational programs. To address this challenge, we have tested a series of supercells with increasing number of atoms (from 30 to 1000) as structural models for ACC. Aiming at elastically isotropic properties of ACC, we analyze the converging size dependence of our results.

MM 54.5 Thu 12:45 TC 006

Natural crash protection: pomelo peels as inspiration for metal foams with improved impact resistance — •Paul Schueler[1], Sebastian Fischer[2], Marc Thielen[3], Thomas Speck[3], Andreas Bührig-Polaczek[2], and Claudia Fleck[1] — [1]Materials Engineering, Institute of Technology, Berlin, Germany — [2]Foundry Institute, RWTH, Aachen, Germany — [3]Plant Biomechanics, University Freiburg, Freiburg, Germany

In biology, structuring often leads to enhanced properties. Inspired by the pomelo peel that exhibits an impact energy dissipation of over 90 % we develop metal based foam structures. Examples for transferred structural principles are sandwich arrangements of foam layers with varying cell sizes that greatly reduce scatter of the strength values, and fibre reinforcements of the foams that locally stabilise cells by redistributing the load. On a lower hierarchical level, we evaluate the influence of strut microstructure and of the strut and cell geome-

try. We combine mechanical testing with different imaging techniques: video recordings allow us to evaluate the foams' macroscopic failure mechanisms during low- and high-speed compression tests, while in situ testing in the SEM or lab/synchrotron micro-CT gives 2D/3D-information on deformation and crack development on the microscale, on cells or single struts deformed to defined strain values. We now better understand the deformation mechanisms of the bio-inspired foam structures at different hierarchical levels as well as the influence and interactions of the single hierarchical levels.

MM 55: Mechanical Properties III

Time: Thursday 11:45–12:45 Location: TC 010

MM 55.1 Thu 11:45 TC 010

Microstructure and Texture in a Cu-Cr Alloy deformed by High Pressure Torsion — •Ksenia Kosyakova[1,2,3], Christine Tränkner[3], Aurimas Pukenas[3], Paul Chekhonin[3], Daria Shangina[1,2], Petr Straumal[1,2], Boris Straumal[2,4], Sergey Dobatkin[1,2], and Werner Skrotzki[3] — [1]A.A. Baikov Institute of Metallurgy and Materials Science of RAS, Moscow, Russia — [2]National University of Science and Technology "MISIS", Laboratory of Hybrid Nanostructured Materials, Moscow, Russia — [3]Institute of Structural Physics, Dresden University of Technology, Dresden, Germany — [4]Institute of Solid State Physics of RAS, Chernogolovka, Russia

The evolution of microstructure and texture in a Cu-0.7%Cr alloy deformed by high-pressure torsion (HPT) was examined depending on shear strain. Disks (diameter 10mm, thickness 0.6mm) were annealed at 600°C for 800h and HPT processed at room temperature under a hydrostatic pressure of 5 GPa for 0.5, 1, 3, 5 and 15 turns (max. shear strains 26, 52, 157, 262, 785). Electron backscatter and X-ray diffraction were applied at half-radius position for microstructure and texture analysis. After 5 rotations, a homogeneous ultrafine-grained structure is found with mean grain size of 190nm and predominance of high-angle boundaries. The texture consists of components typical for fcc-metals processed by simple shear deformation. Moreover, a new {1-14}<110> component is observed which is the main component for all shear strains. After 5 turns, the intensities of all components stay approximately the same.

MM 55.2 Thu 12:00 TC 010

Formation of Oblique Cube Component in Intermetallic Compounds Deformed by High Pressure Torsion — •Christine Tränkner[1], Aurimas Pukenas[1], Jelena Horky[2], Michael Zehetbauer[2], and Werner Skrotzki[1] — [1]Institute of Structural Physics, Dresden University of Technology, Dresden, Germany — [2]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Vienna, Austria

NiAl, YCu and TiAl polycrystals with B2 and $L1_0$ structure, respectively, have been deformed by high pressure torsion at temperatures between 20°C and 500°C at a hydrostatic pressure of 8 GPa to high shear strains. Local texture measurements were done by diffraction of high-energy synchrotron radiation and X-ray microdiffraction. In addition, the microstructure was analyzed by electron backscatter diffraction. Besides typical shear components an oblique cube component is observed with quite large rotations about the transverse direction. Based on the temperature dependence of this component as well as to microstructure investigations it is concluded that it is formed by discontinuous dynamic recrystallization. The influence of high pressure on recrystallization of intermetallics at low temperatures is discussed.

MM 55.3 Thu 12:15 TC 010

Hot Isostatic Pressed Tungsten Fiber-Reinforced Tungsten — •Bruno Jasper[1], Jan W. Coenen[1], Johann Riesch[2], Till Höschen[2], and Christian Linsmeier[1] — [1]Forschungszentrum Juelich GmbH, IEK4 - Plasmaphysik, 52425 Jülich, Germany — [2]Max-Planck-Institut für Plasmaphysik, 85748 Garching, Germany

Tungsten fiber-reinforced tungsten (W_f/W) is a composite material that addresses the brittleness of tungsten (W) at low temperatures and after operational embrittlement, through extrinsic toughening by introducing crack energy dissipation mechanisms. Existing W_f/W samples produced via chemical vapor infiltration indeed showed higher toughness in mechanical tests than pure W. In this contribution W_f/W material specimens produced via powder metallurgical (PM) methods, e.g. hot isostatic pressing (HIP), are shown. A variety of measurements, e.g. 3-point bending and push-out tests, are presented to verify the operation of the expected toughening mechanisms. Therefore the focus of the investigations lies on the interface deboning behavior. In particular, the stability and integrity of the interface is investigated, since high temperatures (up to 1900 °C) and pressures (200 MPa) are present during the composite preparation. First HIP single-fiber samples indicate a compact matrix with densities of 99+ % of the theoretical density of W and showed signs of recrystallization and grain growth. SEM analysis demonstrates an intact interface with indentations of powder particles at the interface-matrix boundary. Push-out test results indicate that the structure of the interface may be damaged by HIPing since push-out of matrix elements is observed.

MM 55.4 Thu 12:30 TC 010

Aluminium-magnesium lightweight metal compound — •Enrico Knauer, Jens Freudenberger, and Ludwig Schultz — IFW Dresden Helmholtzstraße 20 01069 Dresden

Although the workability of magnesium is negligible under the conditions of rotary swaging, co-deformation of magnesium within a tube is possible. This process can be operated successfully up to a logarithmic deformation strain of at least 8, when utilizing an AA6082 tube. The microstructure of magnesium shows a decreasing grain size with increasing deformation strain, saturating at a grain size well below 5 *m. In addition, a preferential texture with a [1 010] ring fibre component is established during deformation. The evolution of the microstructure determines the mechanical properties of the composite, which is characterised by an ultimate tensile strength of 240 MPa. This corresponds to a specific strength of 104 MPa/(g/cm3).

MM 56: Focused Session on GHz Dielectrics: Materials for Mobile Communication II (jointly with HL, MM, DY)

Organizer: Martin Letz (Schott AG Mainz)

Time: Thursday 15:00–17:00 Location: EB 407

Topical Talk MM 56.1 Thu 15:00 EB 407

Temperature stable low loss ceramics for resonators and filters — •Ian Reaney — Materials Science and Engineering, University of Sheffield, Sheffield, UK

Micro wave (MW) dielectric ceramics are required to be temperature stable and have a low dielectric loss to prevent heating of the sample when operated at or near resonance. They are used in many applications but specifically in this contribution the use of MW dielectric ceramics as resonators, filters and antennas is considered. The relevant technologies for these application are reviewed along with their selective materials parameters. The underpinning crystal chemistry that leads to optimisation of properties is also reviewed and some new materials and novel processing routes to improve device performance are discussed.

MM 56.2 Thu 15:30 EB 407

Titanate-based paraelectric glass-ceramics for applications in GHz electronics — •Hubertus Braun[1,2,3], Martin Letz[2], Martun Hovhannisyan[2], and Hans-Joachim Elmers[1] — [1]Johannes-Gutenberg Universität Mainz — [2]SCHOTT AG, Mainz — [3]Graduate School Materials Science in Mainz

In the current work, titanate-based glass-ceramics ($TiO_2 > 45$ mol %) in the La_2O_3-TiO_2-SiO_2-B_2O_3 system are developed ($\varepsilon_r \approx$ 20-30, Qf $\approx$ 10.000 GHz, $|\tau_f| < 10$ ppm/K) which show promising properties as microwave materials and offer numerous advantages in comparison to conventional sintered ceramics. Glass-ceramics which are obtained via a true glassy phase are comparatively new in this field and will be presented as suitable alternative. Glass-ceramics are produced in a two step process: At first, a basic glass is casted in a conventional glass production process. Then the glass undergoes a temperature treatment with a defined temperature profile to initiate a controlled partial crystallization of desired paraelectric phases inside the glassy matrix. Obtaining materials via a homogeneous glassy phase enables intrinsically pore-free materials with comparatively superior surface properties. The effect of solid solution type doping on the dielectric properties and glass stability is investigated. The effect of solid solution type doping on the A(La) and B(Ti) site of the crystalline phases with ions of similar ionic radius is investigated concerning their influence on the dielectric properties and glass stability. Further the materials are analyzed concerning suitability for dielectric loaded antenna applications.

MM 56.3 Thu 15:50 EB 407

Microwave electric properties of thin-film $Ba_xSr_{1-x}TiO_3$ varactors with highly-conducting epitaxial $SrMoO_3$ oxide electrodes — •Arzhang Mani[1], Aldin Radetinac[1], Mohammad Nikfalazar[2], Sergiy Melnyk[2], Philipp Komissinskiy[1], Yuliang Zheng[2], Rolf Jakoby[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Deutschland — [2]Institut für Mikrowellentechnik und Photonik, Technische Universität Darmstadt, 64283 Darmstadt, Deutschland

We present high-frequency properties of MIM thin-film varactors with dielectric $Ba_xSr_{1-x}TiO_3$ (x = 0.4, 0.5, 0.6). Single crystalline $Ba_xSr_{1-x}TiO_3$ layers were grown epitaxially on highly-conducting oxide $SrMoO_3$ electrodes with room-temperature resistivity of 30 $\mu\Omega\cdot$cm. Au/Pt top electrodes were deposited by magnetron sputtering on top of the $Ba_xSr_{1-x}TiO_3$ / $SrMoO_3$ heterostructures and patterned with photolithography and lift-off. Influence of Ba content (x), thickness of $Ba_xSr_{1-x}TiO_3$ layer, and size of the top electrodes on performance of the varactors were investigated in the frequency range of 100 MHz to 10 GHz. Capacitance of 15 pF, quality factor of 15, and tunability of 40% at 0.3 MV/cm were obtained at 100 MHz. The obtained results suggest a high potential of the oxide perovskite electrode material $SrMoO_3$ [1] for fabrication of highly tunable varactors in microwave applications.

[1] A. Radetinac *et al.*, Appl. Phys. Lett. **105**, 114108 (2014).

MM 56.4 Thu 16:10 EB 407

Continuously tuneable, high performance phase shifters based on liquid crystal for applications in phased array antennas — •Matthias Jost, Christian Weickhmann, and Rolf Jakoby — Institute of Microwave Engineering and Photonics, Technische Universität Darmstadt, Merckstr. 25, 64283 Darmstadt, Germany

During the last decade, calamitic-nematic liquid crystals (LCs), well-known from the LC-display technology (LCD), have become increasingly popular in the field of microwave engineering. Due to their unique property of exhibiting local anisotropy, they offer the possibility of realising passive, continuously tuneable devices, such as phase shifters, tuneable filters, polarisers or matching networks. LC can be oriented continuously between the two extreme states (parallel or perpendicular to an applied RF field), either by applying a magneto-static or an electro-static field. Depending on the orientation of the LC, its permittivity and dielectric loss changes. This work presents the recent progress of our research in the topic of hollow waveguide based LC phase shifters for application in phased array antennas. This kind of phase shifter is suitable for high performance applications due to its high figure of merit (FoM), defined by the ratio of the maximum differential phase shift over the highest insertion loss in all tuning states. Full wave simulation results as well as measurement results of realised phase shifters will be shown and a perspective of a phased array antenna for satellite communication will be given.

Topical Talk MM 56.5 Thu 16:30 EB 407

Low loss flexible and stretchable dielectrics for microwave applications — •Mailadil Sebastian — Department of Electrical Engineering, University of Oulu, 90014 Oulu

Flexible, bendable and stretchable dielectrics which can cover even curved surfaces are important for applications in electronic control systems, consumer electronics, heart pacemakers, body worn antenna etc. The requirements for a material to be used as a flexible dielectric waveguide are mechanical flexibility, high relative permittivity, low dielectric loss, high thermal conductivity, low coefficient of thermal expansion (CTE) etc. It is very difficult to identify a single material which possesses all these properties simultaneously. There are a number of ceramic materials with high relative permittivity and low dielectric loss but are brittle in nature. Butyl and silicone rubbers have low loss with good mechanical flexibility and stretchability but they have low relative permittivity and high CTE. Therefore, the practical applications of a rubber or a ceramic alone is limited. By integrating the flexibility, stretchability and low processing temperature of a rubber with high relative permittivity and low loss of ceramics, a composite may be formed, which can deliver improved performances. In this talk the effect of addition of several ceramics such as SiO_2, Al_2O_3, TiO_2, $Ba(Mg_{1/3},Ta_{2/3})O_3$, $Ba(Zn_{1/3},Ta_{2/3})O_3$, $BaTiO_3$, $Ba_{0.7}Sr_{0.3}TiO_3$, $SrTiO_3$, AlN, $Sr_2Ce_2Ti_5O_{15}$ in butyl and silicone rubbers on the microwave dielectric properties, thermal conductivity, thermal expansion, moisture absorption, mechanical properties etc will be discussed.

MM 57: Frontiers of Electronic Structure Theory: Many-body Effects on the Nano-scale

Time: Friday 9:30–12:15 Location: H 0105

Invited Talk MM 57.1 Fri 9:30 H 0105

Excitations and charge transfer phenomena in C based systems — •Elisa Molinari — University of Modena and Reggio Emilia, Modena, Italy — CNR, Istituto Nanoscienze, Modena, Italy

Excitonic effects control excitations and optical spectra in graphene-based nanostructures and related polymers [1], as well as in interacting C-based molecular systems of relevance for photovoltaics [2]. I will show results from ab-initio many body perturbation theory and discuss their implications for spectroscopies and for a realistic description of ultrafast charge separation phenomena.

[1] R. Denk et al, Nat Commun 5, 4253 (2014); A. Batra et al, Chem Sci 5, 4419-4423 (2014); L. Massimi et al, J. Phys. Chem C, in press. [2] S. M. Falke et al, Science 344, 1001-1005 (2014).

Invited Talk MM 57.2 Fri 10:00 H 0105

Towards optimal correlation factors for many-electron perturbation theories — •Andreas Grüneis — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — Universität Wien, Vienna, Austria

Many electron perturbation theories such as the coupled-cluster method form a hierarchy of increasingly accurate approximations to the electronic ground state wave function. This presentation will overview recent progress in applying coupled-cluster methods to solids and techniques to reduce their computational cost such as explicit correlation methods [1,2]. Furthermore applications to archetypal solid state systems as well as the uniform electron gas model system will be discussed [3].

[1] G. H. Booth, A. Grüneis, G. Kresse and A. Alavi, Nature 493, 365-370 (2013).

[2] A. Grüneis, J.J. Shepherd, A. Alavi, D.P. Tew, G.H. Booth, The Journal of chemical physics 139 (8), 084112 (2013).

[3] J.J. Shepherd, A. Grüneis, Physical Review Letters 110 (22), 226401 (2013).

Invited Talk MM 57.3 Fri 10:30 H 0105

Towards an ab-initio description of high temperature superconductivity — •Garnet Chan — Department of Chemistry, Princeton University, United States NJ08544

I will describe our continued efforts in developing ab-initio many-body theory in the condensed phase with a view to a first principles description of a cuprate phase diagram.

Coffee break

Invited Talk MM 57.4 Fri 11:15 H 0105

Correlation effects in unconventional superconductors: from micro- to nano- and macroscales. — •Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

The combination of ab initio density functional theory with dynamical mean field theory (DFT+DMFT) has been proven to be a powerful approach for describing correlation effects in solid state systems at the microscopic level. In this talk we will focus on recent progress on this method and its application to unconventional superconductors such as Fe-pnictides, organic charge-transfer salts as well as correlated Dirac metals [1,2,3]. Further, we shall discuss the manifestation of such effects at the nano- and macroscales.

[1] I. I. Mazin *et al.* Nature Communications 5, 4261 (2014)
[2] S. Backes *et al.* New J. Phys. 16, 083025 (2014)
[3] J. Ferber *et al.* Phys. Rev. B 89, 205106 (2014)

Invited Talk MM 57.5 Fri 11:45 H 0105

Stochastic density functional and GW theories scaling linearly with system size — •Roi Baer[1], Daniel Neuhauser[2], and Eran Rabani[3] — [1]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, 91904 Israel. — [2]Department of Chemistry and Biochemistry, University of California, Los Angeles Los Angeles, CA 90095-1569 USA. — [3]Department of Chemistry, University of California, Berkeley, Berkeley, CA 94720 USA.

Kohn-Sham density functional theory (KS-DFT) is formulated as a statistical theory in which the electron density is determined from an average of correlated stochastic densities in a trace formula. Method allows reliable estimates of the electronic band structure, forces on nuclei, density and moments etc. "Self-averaging" leads to sublinear scaling. An embedded fragment stochastic DFT greatly decreases statistical fluctuations. Based on stochastic DFT a GW method is developed scaling linearly with system size. We demonstrate the results on silicon nanocrystals and large water clusters. References: *Phys. Rev. Lett. 111, 106402 (2013). *Phys. Rev. Lett. 113, 076402 (2014). *J. Chem. Phys. 141, 041102 (2014).