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Overview of Invited Talks and Sessions

(Lecture rooms: BAR 205, IFW A, IFW B, IFW D, and BAR Schön; Posters: P4)

Invited Talks

MM 1.1	Mon	9:30–10:00	BAR 205	Progress in understanding nanoscale plasticity using quantitative in situ TEM — ●DANIEL KIENER
MM 12.1	Mon	15:00–15:30	BAR 205	Building Thermodynamic Models Made Easy: A Bayesian Compressing Sensing Approach to Automatically Cluster-Expanding 1500 Alloy Systems — ●GUS L. W. HART, LANCE J. NELSON, CONRAD W. ROSENBROCK, FEI ZHOU, VIDVUDS OZOLINS
MM 19.1	Tue	9:30–10:00	BAR 205	Size effects on ion transport and energy storage in nanomaterials — ●JOACHIM MAIER
MM 29.1	Tue	15:00–15:30	BAR 205	Grain boundaries in metals: phase and structure transitions studied by tracer diffusion — ●SERGIY DIVINSKI
MM 35.1	Wed	9:30–10:00	BAR 205	From grain boundary premelting to liquid metal embrittlement: A modelling perspective — ●ROBERT SPATSCHEK
MM 47.1	Thu	9:30–10:00	BAR 205	Coherent X-ray Diffraction Imaging of Excitations in Metal Nanoparticles — ●IAN ROBINSON
MM 57.1	Thu	15:00–15:30	BAR 205	Toward the development of Dy-free high coercivity Nd-Fe-B permanent magnets — ●KAZUHIRO HONO, HOSSEIN SEPEHRI-AMIN, TADAKATSU OHKUBO
MM 63.1	Fri	9:30–10:00	BAR 205	Water induced deformation of nanoporous materials — ●OSKAR PARIS

Sessions

MM 1.1–1.1	Mon	9:30–10:00	BAR 205	Invited Talk (Hauptvortrag) Kiener
MM 2.1–2.4	Mon	10:15–11:30	BAR 205	Topical Session: Nanomechanics of nanostructured materials and systems I - Grain size effects
MM 3.1–3.5	Mon	10:15–11:30	IFW A	Functional Materials I - Energy storage
MM 4.1–4.5	Mon	10:15–11:30	IFW D	Computational Materials Modelling I - High throughput/Material discovery
MM 5.1–5.8	Mon	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale (O with HL/TT/MM)
MM 6.1–6.4	Mon	10:15–11:15	IFW B	Microstructure and Phase Transformations I - Martensitic phase transformations
MM 7.1–7.7	Mon	10:45–12:30	POT 081	Energy materials: Water splitting, batteries, and supercapacitors (HL with MM/CPP)
MM 8.1–8.4	Mon	11:45–13:00	BAR 205	Topical Session: Nanomechanics of nanostructured materials and systems II - Thin films
MM 9.1–9.4	Mon	11:45–12:45	IFW A	Functional Materials II - Oxides and Alloys
MM 10.1–10.6	Mon	11:45–13:15	IFW D	Computational Materials Modelling II - Theory/Numerics

MM 11.1–11.6	Mon	11:30–13:00	IFW B	Microstructure and Phase Transformations II - Nucleation/Solidification
MM 12.1–12.1	Mon	15:00–15:30	BAR 205	Invited Talk (Hauptvortrag) Hart
MM 13.1–13.6	Mon	15:45–17:45	BAR 205	Topical Session: Nanomechanics of nanostructured materials and systems III - Small scale plasticity
MM 14.1–14.6	Mon	15:45–17:15	IFW A	Functional Materials III - Li ion batteries
MM 15.1–15.7	Mon	15:45–17:45	IFW D	Computational Materials Modelling III - Bulk thermodynamics/ Phase Transitions I
MM 16.1–16.6	Mon	15:45–17:15	IFW B	Microstructure and Phase Transformations III - Precipitation hardening/ Alloying elements
MM 17.1–17.10	Mon	16:00–18:45	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II (O with HL/TT/MM)
MM 18.1–18.39	Mon	18:00–20:00	P4	Poster Session
MM 19.1–19.1	Tue	9:30–10:00	BAR 205	Invited Talk (Hauptvortrag) Maier
MM 20.1–20.5	Tue	10:15–12:00	IFW A	Topical Session: Nanomechanics of nanostructured materials and systems IV - Tribology/Composites
MM 21.1–21.4	Tue	10:15–11:30	BAR 205	Topical Session: Thermodynamics at the nano scale I - Kinetics, nucleation, grain growth, segregation
MM 22.1–22.6	Tue	10:15–11:45	IFW B	Mechanical properties I - Plastic deformation & fracture
MM 23.1–23.5	Tue	10:15–11:30	IFW D	Electron Microscopy I - Nanomaterials
MM 24.1–24.9	Tue	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III (O with HL/TT/MM)
MM 25.1–25.4	Tue	11:45–13:00	BAR 205	Topical Session: Thermodynamics at the nano scale II - Thermodynamics
MM 26.1–26.5	Tue	11:45–13:00	IFW D	Computational Materials Modelling IV - Phase transitions II
MM 27.1–27.5	Tue	11:45–13:00	IFW B	Transport I - Materials/Methods
MM 28.1–28.5	Tue	12:00–13:15	IFW A	Nanomaterials I - Synthesis of advanced nanostructures
MM 29.1–29.1	Tue	15:00–15:30	BAR 205	Invited Talk (Hauptvortrag) Divinski
MM 30.1–30.6	Tue	15:45–17:45	BAR 205	Topical Session: Thermodynamics at the nano scale III - Novel experimental and theoretical approaches
MM 31.1–31.5	Tue	15:45–17:00	IFW D	Mechanical properties II - Characterisation mechanics
MM 32.1–32.4	Tue	15:45–16:45	IFW B	Transport II - Microstructure/Grain boundaries
MM 33.1–33.7	Tue	15:45–17:45	IFW A	Nanomaterials II - Tubular nanostructures
MM 34.1–34.40	Tue	18:00–20:00	P4	Poster Session
MM 35.1–35.1	Wed	9:30–10:00	BAR 205	Invited Talk (Hauptvortrag) Spatschek
MM 36.1–36.4	Wed	10:15–11:45	BAR 205	Topical Session: Thermodynamics at the nano scale IV - Electrochemistry and strain
MM 37.1–37.4	Wed	10:15–11:15	IFW D	Computational Materials Modelling V - Point defects
MM 38.1–38.6	Wed	10:15–11:45	IFW B	Structural materials
MM 39.1–39.5	Wed	10:15–11:30	IFW A	Liquid and Amorphous Metals I - Shearbands
MM 40.1–40.10	Wed	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV (O with HL/TT/MM)
MM 41.1–41.6	Wed	11:30–13:00	IFW D	Computational Materials Modelling VI - Dislocations
MM 42.1–42.4	Wed	12:00–13:00	IFW B	Electron Microscopy II - Advances in characterisation
MM 43.1–43.5	Wed	11:45–13:00	IFW A	Liquid and Amorphous Metals II - Mechanical properties
MM 44.1–44.5	Wed	15:15–19:00	BAR Schön	Festsitzung zum 50jährigen Bestehen der AG MM / Celebrating the 50th anniversary of the AG MM
MM 45.1–45.11	Wed	16:00–19:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V (O with HL/TT/MM)
MM 46	Wed	19:00–20:00	BAR 205	Mitgliederversammlung des Fachverbands Metall- und Materialphysik
MM 47.1–47.1	Thu	9:30–10:00	BAR 205	Invited Talk (Hauptvortrag) Robinson
MM 48.1–48.5	Thu	10:15–11:30	BAR 205	Topical session: X-ray and neutron scattering in materials science I - Coherent X-ray Diffraction Imaging of Excitations in Metal Nanoparticles

MM 49.1–49.6	Thu	10:15–11:45	IFW D	Computational Materials Modelling VII - Grain boundaries & Interfaces
MM 50.1–50.7	Thu	10:15–12:00	IFW B	Mechanical properties III - Evolution & deformation of microstructure
MM 51.1–51.4	Thu	10:15–11:15	IFW A	Liquid and Amorphous Metals III - Electronic properties of amorphous alloys
MM 52.1–52.10	Thu	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI (O with HL/TT/MM)
MM 53.1–53.5	Thu	11:45–13:15	BAR 205	Topical session: X-ray and neutron scattering in materials science II - Atomic migration studies ranging from neutrons to coherent X-rays
MM 54.1–54.4	Thu	12:00–13:00	IFW D	Computational Materials Modelling VIII - Functional materials
MM 55.1–55.5	Thu	12:00–13:15	IFW B	Nanomaterials III - Electronic, magnetic and optical properties
MM 56.1–56.6	Thu	11:30–13:00	IFW A	Liquid and Amorphous Metals IV
MM 57.1–57.1	Thu	15:00–15:30	BAR 205	Invited Talk (Hauptvortrag) Hono
MM 58.1–58.5	Thu	15:45–17:15	BAR 205	Topical session: X-ray and neutron scattering in materials science III - Real-time insights into fast heat treatment processes using diffraction methods
MM 59.1–59.7	Thu	15:45–17:45	IFW D	Computational Materials Modelling IX - Ferroelectrics
MM 60.1–60.5	Thu	15:45–17:00	IFW B	Nanomaterials IV - Deformation and mechanical properties
MM 61.1–61.6	Thu	15:45–17:15	IFW A	Liquid and Amorphous Metals V - Structure and structure formation
MM 62.1–62.4	Thu	17:30–18:45	BAR 205	Topical session: X-ray and neutron scattering in materials science IV - High Energy Single Grain Diffraction
MM 63.1–63.1	Fri	9:30–10:00	BAR 205	Invited Talk (Hauptvortrag) Paris
MM 64.1–64.4	Fri	10:15–11:30	BAR 205	Topical session: X-ray and neutron scattering in materials science V - X-ray Nanodiffraction Characterization of Inhomogeneous Structural and Mechanical Properties of Thin Films
MM 65.1–65.4	Fri	11:45–13:00	BAR 205	Topical session: X-ray and neutron scattering in materials science VI - Which orientations can we expect for elongated particles in self-confined systems?

Topical session “X-ray and neutron scattering in materials science”

Organizers: Univ.-Prof. Dr. Oskar Paris (Montanuniversität Leoben), Prof. Dr. Martin Müller (Helmholtz-Zentrum Geesthacht)

X-ray and neutron scattering methods have been well-established and inevitable tools to unravel the structure of materials at the nanometer and atomic scale for many decades. Modern synchrotron radiation sources provide a wealth of novel, previously unavailable techniques such as for instance micro- and nanobeam X-ray scattering or the use of coherent X-ray beams that allow reconstructing real space images and 3D strain distribution with nanometer resolution from a scattering experiment. Neutron scattering on the other hand continues to be an extremely useful and complementary tool to enter deep in the bulk of engineering components or to sense magnetism. This symposium aims at bringing together method developers and “users” from all fields of materials research, spanning the range from engineering components to functional nanomaterials.

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:00–20:00 BAR 205

MM 1: Invited Talk (Hauptvortrag) Kiener

Time: Monday 9:30–10:00

Location: BAR 205

Invited Talk MM 1.1 Mon 9:30 BAR 205
Progress in understanding nanoscale plasticity using quantitative in situ TEM — •DANIEL KIENER — Montanuniversität Leoben, Austria

It is established that deformation mechanisms are subject to change once microstructural features approach the micron and sub-micron range [1]. Moreover, miniaturized sample dimensions themselves can lead to pronounced size effects on material strength [2], even if only simple dislocation plasticity governs the plastic deformation.

Quantitative testing in the scanning or transmission electron microscope offers a versatile way to aid to a better understanding of the basic

governing deformation processes, since a direct correlation between the material microstructure or individual crystal defects with the sample deformation behavior and the mechanical properties is achieved by direct observation of the plastic deformation.

In this presentation, different case studies will be presented to highlight recent developments in the field of quantitative nanomechanical in situ testing in the electron microscope, focusing on advanced testing techniques providing novel insights on nanoscale plasticity.

References: [1] T. Zhu, and J. Li: Ultra-strength materials. *Prog. Mater. Sci.* 55, 710 (2010) [2] M. D. Uchic, D. M. Dimiduk, J. N. Florando, and W. D. Nix: Sample Dimensions Influence Strength and Crystal Plasticity. *Science* 305, 986 (2004)

MM 2: Topical Session: Nanomechanics of nanostructured materials and systems I - Grain size effects

Time: Monday 10:15–11:30

Location: BAR 205

Topical Talk MM 2.1 Mon 10:15 BAR 205
Effects of grain size, alloying and temperature on the mechanical behavior of nanocrystalline metals — •RUTH SCHWAIGER — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-WBM)

Characterization, control and optimization of mechanical properties are key issues in materials engineering. While nanocrystalline metals are very attractive candidates for applications requiring high strength, size-dependent deformation, deformation mechanisms and microstructural stability are still under debate. Experimentally, the transition from bulk to interface-dominated deformation mechanisms in nanocrystalline metals is reflected by increased strain rate sensitivity at low temperatures and smaller activation volumes compared to coarse-grained materials. Introducing miscible solutes can be expected to lead to modified mechanical properties compared to the pure metals. Furthermore, alloying of nanocrystalline metals may stabilize the microstructure if the solute segregates to the boundaries facilitating mechanical testing at elevated temperatures. Our investigations of PdAu and PdAg alloys showed a hardness increase with increasing alloying content. The grain size was observed to increase with increasing plastic strain at room temperature while the grain size was stable at annealing temperatures up to 95°C. In this presentation, mechanical behavior and size effects will be discussed for different metallic alloying systems and grain sizes.

MM 2.2 Mon 10:45 BAR 205
Nanoindentation of sputter-deposited Al and Al-Li thin films — •DIANA COURTY, ALLA S. SOLOGUBENKO, and RALPH SPOLENAK — Laboratory for Nanometallurgy (LNM), ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich, Switzerland

Bulk, heavily-deformed fine-grained Al-Li-based alloys are known for their superplastic behavior at elevated temperatures. In these materials, grain-rotation is considered to be the major mechanism responsible for large plastic strains (up to 700%). An intrinsic feature of a thin metallic film, the nano-grained morphology, is very advantageous for the activation of this deformation mode, provided the inherent columnarity of the film morphology can be overcome.

Al- x at.%Li ($x=0, 2, 5,$ and 10) thin film alloys have been sputter-deposited on Si wafers by different sputtering modes enabling the control of the grain morphology, breaking the columnar grain growth and tuning the sublayer thickness. These thin film alloys have been tested by nanoindentation at room temperature, 100°C and 150°C, showing a decrease in hardness for higher indentation temperatures. An effect of film thickness, composition and microstructure on the mechanical behavior of the thin film alloys was studied. Our particular interest is directed to the comparison of films of same thickness and composition but with different grain sizes, were smaller grain sizes showed an increase in hardness - smaller than expected by the Hall-Petch-effect.

MM 2.3 Mon 11:00 BAR 205
Small scale deformation of Chromium - Influence of Microstructure & Temperature — •VERENA MAIER, MEGAN J.

CORDILL, and DANIEL KIENER — Department Materials Physics, Montanuniversität Leoben, Jahnstr.12, A-8700 Leoben

Time-dependent mechanical behavior, expressed by a materials strain-rate sensitivity, is an important indication for thermally activated processes during deformation. The ongoing miniaturization of components and material phases requires studying these effects on the local scale. In this work, the influence of microstructure and temperature on the strain-rate sensitivity of body-centered cubic Cr was studied by nanoindentation strain-rate jump tests at ambient and elevated temperatures. It was observed that Cr in the single crystal condition exhibits a more pronounced strain-rate sensitivity than ultrafine-grained Cr. This is due to the effects of the high lattice friction of bcc-metals at low temperatures, where the motion of the screw dislocations are dominating the deformation behavior, causing there an enhanced strain-rate sensitivity. Increasing the temperature over a material-dependent critical temperature T_c , it is demonstrated that the deformation behavior clearly changes. The thermally activated strength contribution diminishes and thus the strain-rate sensitivity is significantly reduced. However, for the ufg-state an increase of the strain-rate sensitivity with increasing temperature can be observed. This might be correlated to thermally activated motion and annihilation of dislocations at grain boundaries, as previously seen in ultrafine grained face centered cubic materials such as Al and Cu.

MM 2.4 Mon 11:15 BAR 205
Stress induced martensitic phase transformation during nanoindentation in NiTi shape memory alloys — •GUILLAUME LAPLANCHE, GUNTHER EGGELER, and JANINE PFETZING-MICKLICH — Institut für Werkstoffe, Ruhr-Universität Bochum, D-44780 Bochum, Germany

NiTi shape memory alloys (SMA) exhibit remarkable functional properties which rely on a stress and/or temperature induced martensitic phase transformation. Our study is motivated by the need to mechanically characterize small NiTi components, such as micromechanical systems like stents and microactuators. In this study, we use a NiTi alloy with specific phase transformation temperatures. In our NiTi alloy, stress induced martensite is stable at room temperature and this allows its post-mortem characterization. We use EBSD to select grains with specific crystallographic surface normals. In those grains, we perform nanoindentation with spherical indenter tips, in order to avoid symmetries others than those of the crystal structure. The topography of the remnant indents were characterized using atomic force microscopy (AFM). The stress induced formation of martensite shows a crystallographic anisotropy which manifests itself in orientation dependent surface patterns. These patterns reflect the well-known symmetries of the cubic crystal lattice and vanish upon heating, when the martensite transforms back to austenite. AFM investigations of the topography of the regions surrounding the remnant indents directly after nanoindentation, reveal that the stress induced formation of martensite results in the formation of crystallographic sink-in regions surrounding the contact.

MM 3: Functional Materials I - Energy storage

Time: Monday 10:15–11:30

Location: IFW A

MM 3.1 Mon 10:15 IFW A

Graphene-based supercapacitors for energy storage under extreme temperature conditions — ●RANJITH VELLACHERI, AHMED AL-HADDAD, WENXIN WANG, HUAPING ZHAO, CHENGLIANG WANG, ZHILIE WANG, and YONG LEI — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) 98693 Ilmenau (Germany)

Graphene-based supercapacitors have been fabricated for energy storage in a very wide range of temperatures. The optimized supercapacitors showed good charge storage capabilities from $-24\text{ }^{\circ}\text{C}$ to $50\text{ }^{\circ}\text{C}$. Specific capacitance of the electrode obtained from charge/discharge measurements was 91 F/g at room temperature (RT) and no considerable change when tested at different temperatures (e.g. 73 F/g and 100 F/g at $-24\text{ }^{\circ}\text{C}$ and $50\text{ }^{\circ}\text{C}$, respectively). Our samples also exhibited outstanding capacitance retention and cyclic stability at different operating temperatures. Extremely low equivalence series resistance (ESR) and charge transfer resistance were confirmed by electrochemical Impedance measurements. Especially, the low ESR could also result in high power density even at low operating temperatures. We believe that our results highlight the great prospective of the graphene-based supercapacitors for the efficient energy storage at extreme environments with a wide range of temperature difference

MM 3.2 Mon 10:30 IFW A

Nano-Engineered Three-Dimensional Core/Shell Nanotube Arrays for Realizing High Performance Asymmetric Supercapacitors — ●FABIAN GROTE, LIAOYONG WEN, HUAPING ZHAO, and YONG LEI — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau

The ongoing technological advances in areas such as electric mobility, consumer electronics, and energy harvesting set new demands for energy storage systems. The next generation of high performance devices requires a strongly enhanced electrochemical performance as well as operating safety, limited environmental impact, and economic viability. In order to fulfill these aims a crucial role is addressed to supercapacitors. Today, the main challenge is to increase the specific energy of supercapacitors without sacrificing specific power. Thereby the development of novel functional nanostructures for energy storage is a key challenge. Hence we nano-engineered a complex 3D electrode material based on free-standing open-ended core/shell nanotube arrays with tailored functions, using anodic aluminum oxide nano-templates and atomic layer deposition. The core provides a well electron transport through the entire electrode matrix and the thin shell guarantees a well utilization of the active electrode material. Importantly, we designed and nanostructured both the negative and positive electrode materials individually, using an innovative material combination of polypyrrole and manganese oxide. It is shown that the asymmetric electrode nature of the prepared supercapacitor device enabled us to increase the cell voltage to 1.7 V , which is a major leap to increase the specific energy.

MM 3.3 Mon 10:45 IFW A

Temperature induced modifications of hydrides in Gd(0001) thin films — ●SARA WANJELIK, SAMUEL KÖNIGSHOFEN, and MATHIAS GETZLAFF — Institute of Applied Physics, University of Düsseldorf

Hydrogen in metals has been of great interest in research for the past few decades. But only few investigations are carried out by imaging techniques with a lateral resolution on the nm-scale. Even less research deals with the initial stage of hydride formation. Here we present STM measurements on thin Gadolinium films grown on a W(110) surface concentrating on the initial steps of hydrogen absorption. Absorption of hydrogen at room temperature results in hydride formation. We

observe plastic deformations due to the larger volume of the hydrides. On the one hand, disk-like islands with a diameter of approximately 3 nm and a height of 0.3 nm occur, while on the other hand there are connected areas formed by ramps. The islands arrange in chains. It has also been observed that a new feature, a triangular shaped structure appears together with the islands. Maps of the differential conductivity prove that it has a different electronic structure. The origin of the island and the other structure is not fully understood and yet a field of open research. Additionally, we will present modifications of these structures induced by increasing temperature up to that point which they vanish at.

MM 3.4 Mon 11:00 IFW A

Hydrophobicity patterning of gas diffusion media for polymer electrolyte fuel cells — ●INDRO BISWAS¹, PAWEŁ GAZDZICKI¹, MARTIN TOMAŠ², and MATHIAS SCHULZE¹ — ¹German Aerospace Center (DLR), Institute of Technical Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany — ²University of West Bohemia, New Technologies Research Centre, Univerzitní 8, 306 14 Plzeň, Czech Republic

Polymer electrolyte fuel cells with their high gravimetric energy density face a water balance problem especially under variable loads, e.g. in automotive conditions: The excess product water needs to be removed from the fuel cell while maintaining a humidified membrane.

The gas diffusion layer, which also provides contact to the electrochemically active components, has to achieve the passive management of the water balance. Heterogeneously hydrophobic gas diffusion media have already shown to be more capable of balancing these opposing requirements than conventional materials. Various methods of patterning gradients of hydrophobicity are applied, like microperforation and laser, focused X-Ray and ion beam irradiation. The modifications are analysed with photoemission and infrared spectroscopy and compared for their performance, applicability and scalability.

The research leading to these results has received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) for Fuel Cell and Hydrogen Joint Technology Initiative under Grant No. 303446 (Impala).

MM 3.5 Mon 11:15 IFW A

NMR Investigations of the Aluminium Substituted Barium Clathrate $\text{Ba}_8\text{Si}_{46}$ — ●MATEJ BOBNAR, IRYNA ANTONYSHYN, MICHAEL WEDEL, DUONG NGUYEN, ULRICH BURKHARDT, YURI PROTS, BODO BÖHME, LIUDMILA MUZICA, RAUL CARDOSO, WALTER SCHNELLE, IGOR VEREMCHUK, MICHAEL BAITINGER, and JURI GRIN — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden

Clathrates are interesting for their thermoelectric properties, due to their high electric and low thermal conductivity. $\text{Ba}_{8-x}\text{Si}_{46}$ is a type I clathrate obtained at $800\text{ }^{\circ}\text{C}$ and at high pressure of $2\text{--}5\text{ GPa}$. The covalently bonded Si atoms form a framework of small, 20 atom, and large, 24 atom, cages that are fully or partially filled by Ba atoms. Some of the Si atoms may be substituted by a number of other atoms, including Al. $\text{Ba}_8\text{Al}_x\text{Si}_{46-x}$ is reported with a homogeneity range of $8 \leq x \leq 15$. Our investigations, however, begin with a clathrate of even lower Al content, $\text{Ba}_8\text{Al}_{6.8}\text{Si}_{39}$ and continue towards the Al-rich phases. We try to determine, which Si atoms are substituted by Al and how a disorder increases or decreases with a growing Al content. Since Al and Si stand next to each other in the periodic table of elements, they are very difficult to discern by X-ray. For this reason, the NMR was employed, which observes local environments of each nucleus separately and gives some hints about the intrinsic properties of the samples. In this work, we present a model for Al and Si distribution in the clathrate I framework based on ^{29}Si and ^{27}Al NMR results.

MM 4: Computational Materials Modelling I - High throughput/Material discovery

Time: Monday 10:15–11:30

Location: IFW D

MM 4.1 Mon 10:15 IFW D

An automated first-principles search for solid-state lithium electrolytes — ●RICCARDO SABATINI and NICOLA MARZARI — Theory and Simulation of Materials, EPFL (CH)

In recent years much attention has been given to high-throughput techniques for materials' discovery and characterization, a complex challenge where state-of-the-art theoretical advancements meet data analytics and automated job management. We present here one of the first high-throughput projects done with our AiiDA framework (Automated Interactive Infrastructure and Database for Atomistic simulations), an open-source infrastructure built for largely automatic materials' design and discovery. Starting from the ICSD database, we build an automatic workflow to compute lithium-ion diffusion with Car-Parrinello molecular dynamics. The database subset of target lithium-containing materials is also ranked by citations number; in descending order, each structure is first optimized with a ground-state variable-cell relaxation, followed by a microcanonical simulation. Several techniques to ensure the quality of the workflow have also been developed and are discussed.

MM 4.2 Mon 10:30 IFW D

High-throughput studies multi-component Ni-rich alloys — ●MICHAELA HÖFLER, SASCHA B. MAISEL, and STEFAN MÜLLER — Institute of Advanced Ceramics, TUHH, 21073 Hamburg, Deutschland

We present high-throughput studies of various Ni-rich alloys (Ni-Al, Ni-Ta, Ni-W, Ni-Ta-W, Al-Ni-W, Al-Ni-Ta, Al-Ni-Ta-W and Al-Ni-Ta-W) based on DFT theory guided by the cluster-expansion method. We present CE Hamiltonians, which accurately describe the ground-state behavior of the binary alloys and discuss ternary ground-state compounds $\text{Al}_7\text{Ni}_{24}\text{W}_1$, $\text{Al}_3\text{Ni}_{12}\text{W}_1$ and $\text{Al}_3\text{Ni}_{12}\text{Ta}_1$ found to be stable in multi-component alloys across a data base of over 600 fully-relaxed DFT superstructures with up to four components. The resulting ground-states structures have substitutional $L1_2$ -type order and release nearly 0.5 meV/atom of enthalpy upon formation. Our findings indicate that ternary γ' -derivates of $\text{Al}_x\text{N}_3\text{Ta}_{1-x}$ and $\text{Al}_x\text{N}_3\text{W}_{1-x}$ stoichiometries are energetically favourable over true quaternary Al-Ni-Ta-W compounds at low temperatures.

MM 4.3 Mon 10:45 IFW D

Solubility of Interstitials in Transition Metals: Knowledge Discovery using High-Throughput *ab-initio* Databases — ●UGUR AYDIN, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

The solubility of hydrogen in metals is decisive for a variety of phenomena incl. hydrogen embrittlement, superabundant vacancy formation and hydrogen storage. In order to design materials with tailored specific solution properties of hydrogen, a detailed knowledge about the interaction of hydrogen with the host metal is desired. We have, therefore, generated a solution enthalpy database by using an in-house developed workbench. Systematically exploring the database the elastic and chemical mechanisms governing solution enthalpies for the complete set of transition metals are derived. Several crystal structures

for the host metal (bcc, fcc and hcp) and interstitial atoms have been compared. The systematic analysis resulted in a universal dependence of ΔH as a function of the lattice constant of the host metal. The trends obtained in this study provide important insights into mechanisms determining the solution enthalpy of interstitials in complex compounds.

MM 4.4 Mon 11:00 IFW D

Atomistic and inverse-analytical modeling of elastic properties of coherent nano-phases — LEI CHEN¹, LI-FANG ZHU¹, ●MARTIN FRIÁK^{1,2}, DUANCHENG MA¹, CHRISTOPH P. RACE^{1,3}, VENKATA S.P.K. BHOGIREDDY¹, ROBERT SPATSCHEK¹, BOB SVENDSEN^{1,4,5}, DIERK RAABE¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Institute of Physics of Materials AS CR, v.v.i., Brno, Czech Republic — ³Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Aachen, Germany — ⁴Materials Science Centre, University of Manchester, Manchester, United Kingdom — ⁵Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Aachen, Germany

Coherent phases precipitating in metallic matrices are known to provide e.g. a significantly increased strength and other superior mechanical properties. Nano-sized inhomogeneities of phases, that exist only when stabilized by the surrounding matrix, represent a very specific sub-class of these composites. The stabilization via internal interfaces is crucial as these phases would be thermodynamically and/or mechanically unstable as self-standing bulk. In our study we suggest the effective merging of these coherent inhomogeneities with their interfaces into a medium that is characterized by anisotropic elastic constants fulfilling conditions of mechanical stability. We combine an inverse analytical method with atomistic simulations in order to predict elastic constants and apply our approach to bcc Cu in ferritic Fe matrix.

MM 4.5 Mon 11:15 IFW D

Three-dimensional structure maps for sp-d-bonded systems — ●ARTHUR BIALON, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Structure maps are an approach to identify the governing factors that determine if a mixture of elements will form a compound and which crystal structure is to be expected. Here, we present new structure maps for the sp-d-bonded systems that are footed on databases of experimentally observed crystal structures. For identifying suitable axes of the structure map we take into account both the overlap of different crystal-structure regions and the clustering of entries representing the same crystal structure. As a result, we find three most significant order parameters, in particular an electron-count, a volume and electronegativity parameter. This enables us to set up a three-dimensional structure map for the most frequently occurring crystal structures in sp-d-bonded systems that correctly predicts the ground state structure in 9 out of 10 cases.

MM 5: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale (O with HL/TT/MM)

Non-equilibrium processes such as charge and heat transport are central to electronic and thermoelectric applications. Understanding these phenomena at the nanoscale challenges both theory and experiment. Basic theoretical issues are related to the role of quantum mechanics, the interplay of ballistic, diffusion and hopping processes, the importance of dissipation, the effect of electronic correlation, and the signatures of unusual quantum states. On the experimental side devising measurements to unravel these phenomena in a controlled way poses severe difficulties. In this regard, optical lattices of cold atoms are emerging as a powerful laboratory to test theoretical models and discover unforeseen phenomena.

This symposium will cover current issues in the field by bringing together scientists working in different specific areas with the aim of fostering interdisciplinary discussion, assessing current theoretical understanding, and indicating future goals with emphasis on electronic structure theory.

Organizers: Roberto Car (Princeton), Kristian S. Thygesen (Lyngby) and Matthias Scheffler (Berlin)

Time: Monday 10:30–13:15

Location: TRE Ma

Topical Talk

MM 5.1 Mon 10:30 TRE Ma

Molecular junction transport: some theoretical and computational considerations — ●MARK RATNER¹ and MATTHEW REUTER² — ¹Chemistry, Northwestern University, Evanston Illinois 60208 USA — ²Chemistry, Northwestern University, Evanston Illinois 60208 USA

Following the development of break junction techniques, and very elegant measurements by many labs worldwide, the understanding of the community for single molecule transport junctions on the experimental side has been very nicely unified. While there are still challenges, interpretations of the transport (and indeed of some second-order response properties) is now quite sophisticated.

There have been major advances in the computational approaches also, and in many cases, computations and measurements can be compared quantitatively. But there are some remaining difficulties in the computational and theoretical approaches, and this talk will discuss a few of them.

The topics addressed will be: single molecule aspects, histograms and their usage, time-dependence of the transport, and ghost transmission and computational accuracy.

MM 5.2 Mon 11:00 TRE Ma

On the description of biased nanocontacts from ab initio — ●STEVEN ACHILLES¹, JÜRGEN HENK¹, MICHAEL CZERNER², CHRISTIAN HELLIGER², and INGRID MERTIG¹ — ¹Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — ²I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

A suitable description of arbitrary shaped and biased nanocontacts is very important for investigating and predicting physical effects of materials on the nanometer scale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under finite bias we extended our Korrington-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for different types of geometries, i.e. planar junctions [3] and embedded real-space clusters [4]. Both implementations include a self-consistent treatment of the electronic structure under external bias using the nonequilibrium density.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995); P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).

[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).

[3] S. Achilles et al., Phys. Rev. B 88 (12), 125411 (2013).

[4] S. Achilles et al., to be published

MM 5.3 Mon 11:15 TRE Ma

Elasticity changes in molecular junctions under bias: an ab-initio study — ●CLOTILDE S. CUCINOTTA¹, MELIN BAI^{1,2}, IVAN RUNGGER¹, SHMIN HOU², and STEFANO SANVITO¹ — ¹School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — ²Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Non-conservative current induced forces are at the origin of a rich variety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H₂-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants. The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] <http://www.smeagol.tcd.ie/SmeagolDownloads.htm>.

riety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H₂-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants. The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] <http://www.smeagol.tcd.ie/SmeagolDownloads.htm>.

MM 5.4 Mon 11:30 TRE Ma

Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing — ●ZEILA ZANOLLI¹ and JEAN-CHRISTOPHE CHARLIER² — ¹Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — ²IMCN, Université catholique de Louvain (UCL), Belgium

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNTs) decorated with transition metal magnetic nanoclusters (NC).

For small cluster sizes (< 1 nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC. Such a huge local magnetic perturbation can be tailored by molecular adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT-NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The *ab initio* simulations demonstrate that the magnetization change due to the absorption of a single C₆H₆ molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT-NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSnano 6 (2012) 10786-10791.

15 min. break

Topical Talk

MM 5.5 Mon 12:00 TRE Ma

Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment — ●JEFFREY B. NEATON — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Recent scanning tunneling microscope-based break-junction experiments of molecular junctions – devices formed by trapping organic molecules between macroscopic metallic electrodes – have reported robust conductance, thermopower, switching behavior, quantum in-

terference effects, spin-filtering phenomena, and even nonlinear effects such as rectification, establishing such junctions as unique and revealing windows into the physics of charge transport at the molecular scale. In this talk, I will summarize a predictive approach to compute and understand the transport properties of molecular junctions with good accuracy. Our approach includes important exchange and correlation effects missing in standard DFT Kohn-Sham junction level alignment, building on self-energy corrections within a GW approximation. Advantages and limitations of our approach will be discussed quantitatively in the context of a direct comparison with recent photoemission and transport measurements. I will also describe applications of this approach to select junctions exhibiting novel trends in conductance, thermopower, and nonlinear IV characteristics, where new physical insight is obtained by relating computed transport phenomena to junction structure and chemistry.

MM 5.6 Mon 12:30 TRE Ma

Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting — ●STEFAN RINGE, HARALD OBERHOFER, SEBASTIAN MATERA, and KARSTEN REUTER — Technische Universität München, Germany

In the context of solar energy conversion the search for new materials for photo-catalytic water splitting has received new impetus. While in general powerful, computational screening approaches are struggling with the complexity of the underlying physical processes at the solid-liquid interface. Recent work points in particular at the necessity to include at least an efficient description of solvent screening effects to compute meaningful descriptors even in simple computational hydrogen electrode approaches. To this end, we present an implementation of the modified Poisson-Boltzmann (MPB) implicit solvation model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. Optimally integrating into this code environment, we solve the MPB equation in a novel approach based on an expansion of the electrostatic potential in the localized basis functions of FHI-aims. In contrast to common numerical multi-grid solvers this approach can directly make use of the optimized integration schemes used to reach self-consistency and removes the need for numerical interpolation between different grids. We demonstrate the approach and its efficiency for a range of molecular test systems, and show first results for catalytic water splitting on gold nano-clusters.

MM 5.7 Mon 12:45 TRE Ma

Towards a combined QM/MM and implicit solvent descrip-

tion of photoelectrochemical processes — ●MARKUS SINSTEIN¹, DANIEL BERGER¹, RAN JIA², VOLKER BLUM³, HARALD OBERHOFER¹, and KARSTEN REUTER¹ — ¹Technische Universität München, Germany — ²Jilin University, P.R. China — ³Duke University, USA

Photoelectrochemical systems are widely explored to drive energy-relevant redox reactions like water splitting or CO₂ reduction. The detailed analysis of the involved elementary processes via first-principles calculations is challenged by the necessity to simultaneously account for the extended semiconductor photocatalyst and the liquid electrolyte. Especially for charge (proton and/or electron) transfer steps traditionally employed periodic boundary condition approaches involve charged supercells with difficult to control finite size errors. To this end, we present a solid state QM/MM embedding approach, in which only a finite cluster model of the photocatalyst surface is treated quantum mechanically and the correct Madelung potential of the periodic system is obtained by embedding into a charge field. For the efficient modeling of photoelectrochemical processes we combine this approach with an implicit solvation scheme within the DFT package FHI-aims. Finally, we also show early test results of the combined QM/MM implicit solvent model.

MM 5.8 Mon 13:00 TRE Ma

Ab-initio Simulation of Molecular Networks on the Surface of Water — ●RALPH KOITZ, MARCELLA IANNUZZI, ARI P SEITSONEN, and JÜRIG HUTTER — University of Zurich, Zurich, Switzerland

Molecules adsorbed on surfaces play an important role in catalysis, surface science, and nanotechnology. Traditionally, research has focused on various adsorbates atop metals and metal oxides using computational and surface-science techniques. More recently, however, it was demonstrated that ordered monolayer networks can also be formed on the surface of liquid water by using metal ions to bind together multidentate precursor molecules. As these assemblies are difficult to characterize, computational methods can provide valuable insight into their formation and structure.

In this contribution we present large-scale DFT-based molecular dynamics simulations of the formation of a network of *tris*-terpyridine-derived molecules (TTPB) on a water slab. In particular, we focus on the structure of the molecule on the surface, the mechanism of Zn²⁺ ion insertion from the solution and the subsequent linking of molecules into aggregates. We employ the metadynamics method to quantify the free energy surface of the involved processes. Our results provide detailed insight into on-surface and subsurface diffusion in this system and chemical reactions of TTPB on the surface of water.

MM 6: Microstructure and Phase Transformations I - Martensitic phase transformations

Time: Monday 10:15–11:15

Location: IFW B

MM 6.1 Mon 10:15 IFW B

Nucleation and growth of martensite in epitaxial magnetic shape memory films — ●ROBERT NIEMANN^{1,2}, ANJA BACKEN¹, HANUŠ SEINER³, SANDRA KAUFFMANN-WEISS^{1,4}, CHRISTIAN BEHLER^{1,2,4}, ULRICH K. RÖSSLER¹, LUDWIG SCHULTZ^{1,2}, and SEBASTIAN FÄHLER^{1,2,4} — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — ²Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — ³Institute of Thermomechanics, ASCR, Dolejškova 1402/5, 182 00 Prague, Czech Republic — ⁴Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Physics, D-09107 Chemnitz, Germany

The complex martensitic microstructure of modulated magnetic shape memory alloys is beneficial for magnetic field induced reorientation or reversible field induced phase transition [1]. The big difference in mobility between type I and type II twin boundaries highlights the importance of a monoclinic description of the lattice. Hence it is important to understand the microstructure from the atomic up to the macroscale. As a model system we analyze the martensitic transformation in epitaxial Ni-Mn-Ga films. We perform temperature dependent SEM imaging during the phase transition and XRD as well as TEM in the martensitic state. We describe the observed stages of nucleation and growth using a crystallographic model based on the Wechsler-Lieberman-Read theory of martensites and finite element methods. [1] R. Niemann et al., Adv. Eng. Mat. 14, 562 (2012)

Supported by SPP1599 www.FerroicCooling.com

MM 6.2 Mon 10:30 IFW B

Composition-dependent atomic positions in Ti-Nb martensites — ●MATTHIAS BÖNISCH^{1,2}, MARIANA CALIN¹, LARS GIEBELER^{1,3}, ARNE HELTH^{1,3}, ANNETT GEBERT¹, WERNER SKROTZKI^{1,2}, and JÜRGEN ECKERT^{1,3} — ¹IFW Dresden, D-01069 Dresden, Germany — ²Technische Universität Dresden, Institute of Structural Physics, D-01069 Dresden, Germany — ³Technische Universität Dresden, Institute of Materials Science, D-01069 Dresden, Germany

In this work the influence of Nb addition on the structural characteristics of martensitic phases in the Ti-Nb system is studied in detail. The orthorhombic martensite alpha' commonly observed in rapidly quenched beta-stabilized Ti-based alloys represents an intermediate structure between the hexagonal martensite alpha' found at low solute content and the bcc beta-phase present at high solute content. While the distortion of the orthorhombic unit cell by addition of beta-stabilizing atoms is well documented in literature, experimental data about the detailed atomic positions in dependence of chemical composition is missing. For this study we prepared a series of binary Ti-Nb alloys by casting techniques followed by homogenization treatment and water quenching. We used X-ray diffraction combined with Rietveld-based analyses to study the gradual structural changes of alpha' and alpha'' martensites effected by addition of Nb and determined their compositional boundaries. In case of orthorhombic alpha'' we found that besides the lattice parameters the locations of atoms on (002)alpha'' planes very sensitively respond to the amount of Nb present.

MM 6.3 Mon 10:45 IFW B

Laser annealing of Fe7Pd3 ferromagnetic shape memory thin films — ●ARIYAN ARABI-HASHEMI¹, MARTIN EHRHARDT¹, PIERRE LORENZ¹, DIETMAR HIRSCH¹, KLAUS ZIMMER¹, and STEFAN G. MAYR^{1,2,3} — ¹Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstraße 15, 04318 Leipzig, Germany — ²Translationszentrum für regenerative Medizin, Universität Leipzig, 04103 Leipzig, Germany — ³Fakultät für Physik und Geowissenschaften, Universität Leipzig, 04103 Leipzig, Germany

Fe7Pd3 is a magnetic shape memory alloy capable of performing strains of up to 5% by applying an external magnetic field. While the austenite phase of Fe7Pd3 is fcc, the martensite phases are fct, bct and bcc. The magnetic shape memory effect is only observed in the fct phase due to a high magnetocrystalline anisotropy and a high mobility of twin boundaries. We study phase transformation effects in Fe7Pd3 films annealed by 25 ns pulses of a KrF laser for various substrates: LaSrAlTaO, MgO and Si. The laser-solid interaction was simulated by finite element method. Laser annealing experiments are compared with thermal annealing experiments. Low temperature electron beam evaporation deposited samples reside in the bcc phase independently of the used substrate. Subsequent laser and thermal annealing of Fe7Pd3 films deposited on MgO reside in the bcc phase, while laser annealed Fe7Pd3 films on LSAT show a phase transformation from bcc to fcc. In thermally annealed Fe7Pd3 on LSAT fcc and fct is observed. Interdiffusion was studied by SIMS.

MM 7: Energy materials: Water splitting, batteries, and supercapacitors (HL with MM/ CPP)

Time: Monday 10:45–12:30

Location: POT 081

MM 7.1 Mon 10:45 POT 081

Highly efficient photocatalytic water splitting with colloidal CdS nanorods by mediated hole scavenging — ●THOMAS SIMON, AURORA MANZI, CHRISTIAN WOLFF, JACEK STOLARCZYK, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität Muenchen, Amalienstr. 54, D-80799

Solar hydrogen production is considered to be as one of the biggest challenges for future energy supply. Colloidal semiconductor nanoparticles, as sunlight absorber with additional noble metal nanoparticles as hydrogen catalyst are well known for photocatalytic hydrogen generation. Many of these systems suffer from low solar to hydrogen efficiencies unless high cost and rare materials like platinum or ruthenium compounds are used as co-catalysts. We demonstrate that it is possible to overcome all these problems with CdS nanorods with a very simple earth-abundant nickel-based co-catalyst. An apparent quantum yield exceeding 50% and long term stability of more than 200h could be achieved. We show that the photocatalytic activity is enhanced ten-fold in highly alkaline environment. Thanks to favourable band alignment the hydroxide anion acts as a redox shuttle relaying the hole from the nanocrystals. Since the hole transfer is considered to be the limiting factor, the quick hole scavenging at high pH is responsible for the enhancement of photocatalytic hydrogen evolution. [1]

[1] T. Simon, M.J. Berr, A. Vaneski, D. Volbers, R. Wyrwich, M. Döblinger, A.S. Susha, A.L. Rogach, F. Jäckel, J.K. Stolarczyk, J. Feldmann, submitted

MM 7.2 Mon 11:00 POT 081

Three-dimensional Ordered Macro-mesoporous Mo:BiVO4 Photoelectrode toward Efficient Photoelectrochemical Water Splitting — ●MIN ZHOU^{1,2}, YANG XU¹, CHENGLIANG WANG¹, LIAOYONG WEN¹, YONG LEI¹, and YI XIE² — ¹Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau, Germany — ²University of Science & Technology of China, Hefei, China

In view of the worldwide energy challenge in the 21st century, the technology of semiconductor-based photoelectrochemical (PEC) water splitting has received considerable attention as an alternative approach for solar energy harvesting and storage. BiVO4 has been regarded as a promising material for PEC water splitting, but it suffers from a major challenge on charge migration. In order to meet this challenge, for the first time, we design a three-dimensional(3D) ordered macro-mesoporous architecture of Mo:BiVO4 through a controllable colloidal crystal template method. Within expectation, a superior photocurrent density is achieved in return for this design. This enhancement origi-

MM 6.4 Mon 11:00 IFW B

Mesoscopic twinning of nanotwinned martensites in epitaxial Ni-Mn-Ga films: A TEM study — ●CHRISTIAN BEHLER^{1,2,3}, ANJA BACKEN¹, HANUŠ SEINER⁴, ROBERT NIEMANN^{1,2}, SANDRA KAUFFMANN-WEISS^{1,3}, LUDWIG SCHULTZ^{1,2}, and SEBASTIAN FÄHLER^{1,2,3} — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — ²Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — ³Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Physics, D-09107 Chemnitz, Germany — ⁴Institute of Thermo-mechanics, ASCR, Dolejškova 1402/5, 182 00 Prague, Czech Republic

Ni-Mn-Ga magnetic shape memory (MSM) alloys have attracted much attention due to the high reversible strains realized by reorientation of martensitic variants by applying external magnetic fields (MIR). To optimize this effect a detailed knowledge about the microstructure is beneficial, since the MIR effect depends on the martensitic phase and the type of mesoscopic twin boundaries connecting the different martensitic variants. As model system epitaxial Ni-Mn-Ga films are investigated which show two different microstructures at the surface. Several cross-sections of both structures were prepared by FIB milling and analyzed by means of (High-Resolution) TEM to gain a complete 3D information about the film structure. We apply a nucleation scenario based on WLR theory to explain the precession of the martensitic transformation for each microstructure. It results in the characteristic formation of mesoscopic twin boundaries we observe in thin films.

nates primarily from effective charge migration according to the analysis of electrochemical impedance spectroscopy. All the results highlight the great significance of the 3D ordered macro-mesoporous architecture as a promising photoelectrode model for the application in solar conversion. The cooperating amplification effects of nanoengineering from composition regulation and morphology innovation provide new opportunities for creating more purpose-designed photoelectrodes with highly efficient performance.

MM 7.3 Mon 11:15 POT 081

Three-dimensional Composite Aerogels and Other Nanostructures for Improved Electrochemical Property — ●LIYING LIANG^{1,2}, YIMENG XU¹, HAIMEI LIU¹, and YONG LEI² — ¹Beijing University of Chemical Technology, State Key Laboratory of Chemical Resource Engineering, 100029 Beijing (PR China) — ²Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Three-dimensional (3D) graphene aerogels possess a lot of unique properties, such as light weight, high conductivity, large surface area, high mechanical strength, and ample volume with hierarchically porous structure, which make them widely applied in various technological fields. Here, 3D porous composite aerogels have been synthesized via an innovative in situ hydrothermal method assisted by freeze-drying process. In this hybrid structure, one-dimensional (1D) AgVO3 nanowires are uniformly dispersed on two-dimensional (2D) graphene nanosheets surfaces or penetrate through the graphene sheets, forming 3D porous composite aerogels. The composite aerogels as cathode materials for lithium-ion batteries, exhibit high discharge capacity, excellent rate capability, and good cycling stability. We are also preparing more novel nanostructures by using AAO templates, which are expected to provide excellent electrochemical performance.

MM 7.4 Mon 11:30 POT 081

Three-dimensional Metal Oxides Based Nano-arrays Anodes for Sodium Ion Batteries — ●YANG XU, MIN ZHOU, HUAPING ZHAO, CHENGLIANG WANG, and YONG LEI — Institute of Physics, Ilmenau University of Technology, 98693 Ilmenau, Germany,

The discovery of new materials/microstructures for electrodes in sodium ion batteries (NIBs) is receiving high levels of scientific attention, as sodium is substantially less expensive and more abundant than lithium. However, there is a limited choice of electrode materials that are suitable hosts to accommodate Na ions and allow for reversible insertion/extraction reactions, since Na ions are 55% larger in radius than Li ions. Of those, most have been identified to be potentially use-

ful as cathodes. On the anode side, hard carbonaceous materials and insertion of Sn, Sb, Pb, and their alloys based anodes have been demonstrated to be highly promising. Another emerging class of materials that remains relatively unexplored in this case is conversion and/or insertion electrodes using transition metal oxides with reasonably low insertion potential. We report the successful utilization combining the nano-structured transition metal oxides and three-dimensional metallic current collector for NIBs anodes, and the results are demonstrated to be promising: the electrodes exhibited a highly stable reversible charge storage capacity over long term cycling, and were able to withstand high rate cycling with fully recovering the initial capacity. This proof-of-principle demonstration opens a way forward for future work on nano-architectures with better NIBs anode performance.

MM 7.5 Mon 11:45 POT 081

First principles study on the electronic properties of NaO₂ — ●MARKUS HEINEMANN¹, PASCAL HARTMANN², CONRAD L. BENDER², PHILIPP ADELHELM², JÜRGEN JANEK², and CHRISTIAN HEILIGER¹ — ¹I. Physikalisches Institut, Justus Liebig University, 35392 Giessen, Germany — ²Physikalisch-Chemisches Institut, Justus Liebig University, 35392 Giessen, Germany

In the light of the recent discovery of rechargeable room-temperature sodium superoxide (NaO₂) batteries [1], a deeper understanding of the electronic properties of NaO₂ has become of broad interest. We investigate the electronic structure of NaO₂ using the framework of density functional theory and employ a hybrid functional approach for the exchange and correlation interaction. The disordered pyrite structure of the NaO₂ room-temperature phase is modeled by taking into account various superoxide orientations in our computations. Our band structure calculations indicate that NaO₂ is an insulator with an energy band gap in the range of 2 eV and that different superoxide alignments lead to a broadening of the conduction band. We compare our calculations to recent experimental investigations on the conductivity of NaO₂.

[1] P. Hartmann, C. L. Bender, M. Vračar, A. K. Dürr, A. Garsuch, J. Janek, and P. Adelhelm, *Nature Mat.* 3486, 1 (2012)

MM 7.6 Mon 12:00 POT 081

Photostability of GaN-metal interfaces in aqueous media — ●CARINA EHRIG^{1,2}, RALF KRAUSE¹, CHRISTOPH BRABEC², and GÜNTER SCHMID¹ — ¹Siemens AG, CT RTC MAT IEC-DE, Erlangen — ²Lehrstuhl für Werkstoffe der Elektronik- und Energietechnik,

FAU Erlangen-Nürnberg, Erlangen

Gallium nitride (GaN) is a well-established semiconductor in optoelectronic applications. It has a wide band gap of 3.4 eV and is thus excitable in the near UV range. A promising application of GaN is its use as a photo electrode driving electrochemical reactions such as photocatalytic water splitting for generation of hydrogen without consumption of fossil fuel or emission of CO₂. The corrosion resistance of those photo electrodes in aqueous media is one of the main factors determining their lifetimes and thus plays an important role for their applicability for highly efficient solar energy conversion. It has been demonstrated in photocatalytic experiments, that under UV-illumination n-type GaN acts as oxygen evolving photo anode and p-type GaN as hydrogen evolving photo cathode.

In the present work, the corrosion resistance of metal-coated n-GaN and p-GaN photoelectrodes in aqueous media is investigated by electrochemical measurements. The influence of an externally applied potential under light excitation as well as the effect of long-term photo-induced stress are studied. It is observed that without illumination the GaN surfaces and GaN-metal interfaces are rather stable, whereas they undergo different corrosion processes when exposed to UV light.

MM 7.7 Mon 12:15 POT 081

Growth and characterization of 3D graphene networks for supercapacitors — ●SIMON DRIESCHNER and JOSE ANTONIO GARRIDO — Walter Schottky Institut, TU München, Am Coulombwall 4, 85748 Garching

The use of graphene as electrode material in supercapacitors has drawn great interest due to a suitable combination of material properties like high surface to volume ratio, high conductivity, and chemical stability. Since the capacitance of one single graphene sheet is rather limited, a continuous 3D network of graphene is expected to enhance the performance of graphene-based supercapacitors. We demonstrate the growth of 3D graphene by chemical vapor deposition (CVD) using a nickel foam as scaffold and a wet-etching transfer, yielding a free-standing macroporous graphene network of high crystalline quality, as shown by Raman spectroscopy. Cyclic voltammetry, charge-discharge measurements, and electrochemical impedance spectroscopy are used to assess the potential of 3D networks of CVD graphene for energy storage applications. We also compare the electronic double layer capacitance of bare graphene foam to the pseudo-capacitance introduced by conductive polymers.

MM 8: Topical Session: Nanomechanics of nanostructured materials and systems II - Thin films

Time: Monday 11:45–13:00

Location: BAR 205

Topical Talk

MM 8.1 Mon 11:45 BAR 205

The Fatigue and Time-Dependent Properties of Freestanding and Supported Thin Gold Films Studied by Bulge Tests — ●BENOIT MERLE and MATHIAS GÖKEN — Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

The bulge test is a method of choice for investigating the mechanical properties of thin films. Its scope was extended to the study of fatigue and time-dependent properties of freestanding and SiNx supported 100 - 400 nm gold films. Fatigue testing is performed by cycling the pressure under the membrane up to 10⁵ times, while the stress and strain in the membrane are continuously measured. Freestanding films experienced a strong ratcheting leading to failure after a few 10⁴ cycles. Observations of the surface showed a sliding of individual grains below the level of the original surface. This grain boundary sliding was obviously eased by the columnar microstructure of the samples. SiNx supported films did neither experience failure nor such strong effects. Only a few abnormally large grains showed extrusions after completion of the fatigue tests. Cyclic creep having been observed for both kinds of samples, creep tests were performed on them. They evidenced widespread grain boundary sliding across the freestanding gold membranes, while this mechanism was prevented by the good adhesion of supported films to their substrate. Strain-rate jump tests showed that this resulted into freestanding gold films having a strain-rate sensitivity 5 times higher than their counterparts bonded to a SiNx substrate.

MM 8.2 Mon 12:15 BAR 205

Fracture Behavior of Freestanding Thin Metal Films Char-

acterized by Bulge Testing — ●EVA PREISS, BENOIT MERLE, and MATHIAS GÖKEN — Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

A bulge test setup was used to perform mechanical tests on rectangular membranes with thicknesses ranging from below 100 nm to 400 nm. From conventional bulge tests, stress-strain curves can be calculated and parameters such as residual stress and plane-strain modulus can be determined. Alternatively, the used setup can be inserted into an atomic force microscope (AFM). During in-situ bulge testing in the AFM the surface of the deforming membrane can be imaged.

In order to determine the fracture toughness of thin films, narrow slits of 10 μm length were milled into the center of the membranes by focused ion beam (FIB). Subsequently, the membranes were loaded until rupture. The fracture toughness obtained for freestanding and supported gold films is far below the fracture toughness reported for bulk gold. By in-situ testing in the AFM out-of-plane motion of individual columnar grains could be revealed as active deformation mechanism in freestanding films.

MM 8.3 Mon 12:30 BAR 205

Mechanical properties of reactively sputtered ceramic single and multilayer thin film structures for dental implants — ●DANIEL MUFF and RALPH SPOLENAK — ETH Zurich, Laboratory for Nanometallurgy, Switzerland

Due to their inherent dark grey color, titanium dental implant screws can cause undesired darkening of the peri-implant mucosa [1]. Ceramic single and multilayer thin film structures have been developed

to increase their reflectance based on interference phenomena.

Besides the esthetic function, the mechanical integrity of the coatings is crucial. As implants bend during chewing motions, coatings have to withstand compressive and, more critically, tensile strains. Therefore, in-situ tensile testing of the ceramic films on polyimide and titanium substrates has been carried out in optical and scanning electron microscopes in order to determine their fracture and delamination behavior.

It was found that the strain at onset of fragmentation decreases with increasing film thickness or number of layers. The crack distance saturates at around 10 times the film thickness and is slightly smaller for coatings on Ti than on polyimide which can be explained by the mismatch of the elastic constants of film and substrate [2]. While buckle formation was observed for thin films, thicker films showed severe delamination.

References: [1] SE Park, JD Da Silva, H-P Weber, S Ishikawa-Nagai (2007) *Clinical Oral Implants Research* 18: 569. [2] ZC Xia, JW Hutchinson (2000) *Journal of the Mechanics and Physics of Solids* 48: 1107.

MM 8.4 Mon 12:45 BAR 205

Influence of the Film Thickness on Fragmentation, Adhe-

sive Failure and Contact Damage of Diamond-Like Carbon (DLC) Coated Titanium Substrates — ●DANIEL BERNOULLI¹, ANDI WYSS¹, KATHRIN HÄFLIGER¹, KERSTIN THORWARTH², GÖTZ THORWARTH³, ROLAND HAUERT², and RALPH SPOLENAK¹ — ¹ETH Zurich - Laboratory for Nanometallurgy, Department of Materials, Zurich, Switzerland — ²EMPA, Swiss Federal Laboratories for Materials Science and Research, Dübendorf, Switzerland — ³DePuy Synthes, Solothurn, Switzerland

Diamond-like carbon (DLC) coated friction pairs are well-known for their long durability and outstanding tribological behavior. However, wear and loose particles trapped between the friction pairs can lead to the appearance of high pressure on the DLC coating and may result in contact damage, fragmentation and adhesive failure. The influence of the DLC film thickness on these three effects is presented in this talk. The contact damage upon indentation was analyzed by finite element analysis and experimental studies. For thicker films circumferential and horizontal cracks are present in the DLC while for thin DLC films pronounced plastic deformation of the substrate occurs. The fragmentation analysis reveals that a very high DLC fracture strength can be achieved by keeping the DLC film thickness $< 1 \mu\text{m}$ and adhesive failure correlates with film thickness and the applied strain. For all three cases an optimal DLC film thickness is presented.

MM 9: Functional Materials II - Oxides and Alloys

Time: Monday 11:45–12:45

Location: IFW A

MM 9.1 Mon 11:45 IFW A

Magnetic characterization and 3D-imaging of epoxy-based magnetocaloric composites — ●BRUNO WEISE¹, BARBARA PULKO², KONSTANTIN SKOKOV³, JAKA TUŠEK², OLIVER GUTFLEISCH³, ANJA WASKE¹, and JÜRGEN ECKERT^{1,4} — ¹IFW Dresden, Institute for Complex Materials, Dresden, Germany — ²University of Ljubljana, Faculty of Mechanical Engineering, Ljubljana, Slovenia — ³TU Darmstadt, Department of Materials Science, Darmstadt, Germany — ⁴Institute of Materials Science, Dresden University of Technology, Dresden, Germany

Epoxy-based magnetocaloric composites of La-Co-Fe-Si with different fractions of active material were produced and characterized. Their magnetic properties, as well as the temperature- and field-dependent specific heat capacity (c_p) were determined. For comparison, a sintered La-Co-Fe-Si and a Gadolinium sample, which is a benchmark material for magnetocaloric materials, was measured. From the specific heat, entropy change ΔS and temperature change, ΔT was calculated and compared with magnetic measurements (ΔS^M) and direct measurements (ΔT^{direct}). Furthermore by using Computed Tomography (CT) exact volume fractions of the active magnetocaloric material, the epoxy and the porosity were studied. We will discuss the magnitude of the magnetocaloric effect with respect to the active magnetic material and the role of the porosity.

MM 9.2 Mon 12:00 IFW A

Interface-related phenomena in coupled direct and inverse magneto-caloric materials: A first-principles study — ●BISWANATH DUTTA, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

A combination of different magneto-caloric materials in a single system gives rise to new phenomena that can be highly relevant for applications. Within this study, we investigate the physical properties of systems containing Ni-Mn-Ga and Ni-Mn-Sn, which show direct and inverse magneto-caloric effect respectively. X-ray diffraction experiments indicate that their combination in a layered structure significantly changes the structural properties of both phases. We have investigated the underlying mechanisms for this observation using density functional theory. On the one hand, our calculations reveal that the atomic magnetic moments get modified near the interface implying that interfaces influence transition temperatures and entropy changes. On the other hand, we have carefully investigated strain contributions, interlayer diffusion as well as defect formation such as vacancies. Our calculated results show clear indications for Ga diffusion into Ni-Mn-

Sn, thereby modifying the chemistry of the alloy. We discuss these results in the framework of lattice expansion and vacancy formation for various species and have used them to explain the experimental observations.

MM 9.3 Mon 12:15 IFW A

Recent progress in development of Fe-Pd ferromagnetic shape memory films and foils for biomedical applications — Y. MA¹, A. ARABI-HASHEMI¹, A. LANDGRAF¹, U. ALLENSTEIN^{1,3}, M. ZINK³, and ●S.G. MAYR^{1,2,3} — ¹Leibniz-Institut für Oberflächenmodifizierung e.V. Leipzig — ²Translationszentrum für regenerative Medizin — ³Fakultät für Physik und Geowissenschaften, Universität Leipzig

Due to their excellent biocompatibility, Fe-Pd based ferromagnetic shape memory alloys are highly promising materials for use as actuators or sensors in biomedical applications. Yet, their application within these areas has been hampered by unresolved issues, including i) synthesis as freestanding single-crystals in the desired fct martensite phase, ii) optimization for a martensite temperature located sufficiently above body temperature, iii) activation of twin boundary motion and iv) mechanical coupling to cells. The present contribution will review recent progress in coping with challenges i)-iv), employing molecular beam epitaxy for single crystal synthesis, ion beam irradiation for tuning martensite transformation, film-lift-off by a tailored etching approach, followed by functionalization with biomolecules for interfacing to cells. In doing so, we particularly focus on the physical understanding, how synthesis parameters affect resulting properties and functionality.

MM 9.4 Mon 12:30 IFW A

Electrical and magnetic properties of Fe-based bulk metallic glass with minor Co and Ni addition — ●HYO YUN JUNG — IFW Dresden, Institute for Complex Materials, D-01069 Dresden, Germany

Effect of minor Co and Ni alloying on soft magnetic properties and electrical resistivity (ρ) of Fe_{75.5}Co_{7.0}Si_{3.3}B_{5.5}P_{8.7} (at.%) bulk metallic glass (BMG) has been investigated. Within examined compositional range (Co and Ni up to 4 at.%), the saturation magnetization (M_s) and ρ of the alloy continuously decrease with increasing Co and Ni contents, while the Curie temperature (T_c) and initial permeability of the alloy increase. Comparing the effect of Co and Ni additions, the alloys with Co addition have much higher T_c and M_s than the alloy with Ni addition. The present results suggest that minor addition of Co can provide better effectiveness to enhance the magnetic softness of Fe-based BMGs than minor Ni addition.

MM 10: Computational Materials Modelling II - Theory/Numerics

Time: Monday 11:45–13:15

Location: IFW D

MM 10.1 Mon 11:45 IFW D

Accurate ab-initio elastic properties at 0K and above: The ElaStic tool — ●JÜRGEN SPITALER¹, ROSTAM GOLESORKHTABAR², PASQUALE PAVONE², CLAUDIA DRAXL², and PETER PUSCHNIG³ — ¹Materials Center Leoben Forschung GmbH, Roseggerstr. 12, 8700 Leoben, Austria — ²Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ³Institut für Physik, Karl-Franzens-Universität Graz, Universitätsplatz 5, 8010 Graz, Austria

Elastic properties are a key for understanding the mechanical behavior of materials. ElaStic [1] greatly facilitates a reliable determination of elastic constants for materials with any lattice type from first-principles. Results for various materials at 0K will be presented, including systems with low symmetry. At the same time, some nuts and bolts of elastic-constant calculations will be discussed. We will show, how the formalism can be extended towards finite temperatures, either implicitly via the lattice expansion, or explicitly by fitting free energy versus strain. Its application will be demonstrated for a prototypical example.

[1] R. Golesorkhtabar, P. Pavone, J. Spitaler, P. Puschnig, and C. Draxl, *Comp. Phys. Commun.* 184 (2013), 1861

MM 10.2 Mon 12:00 IFW D

KKRnano: DFT for nano-scale systems — ●ELIAS RABEL, RUDOLF ZELLER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

The screened KKR Green's function method has been implemented in our code KKRnano [1] for all-electron DFT calculations of unit cells containing thousands of atoms. KKRnano has been successfully applied in the study of phase-change materials and dilute magnetic semiconductors. The KKR method considers multiple scattering of partial waves up to a maximal angular momentum ℓ_{\max} . Motivated by the idea that at long-range low ℓ -components dominate the scattering, we employ a distance dependent angular momentum cut-off of the Green's function to reduce the effective matrix size with little compromise in accuracy. The special case of neglecting all partial waves scattered from reasonably large distances leads to an $O(N)$ -scaling method. Combining this approach with the capacities of present day supercomputers, DFT calculations of more than 100000 atoms become technically feasible. The question of attaining sufficiently accurate, self-consistent solutions has to be addressed. We present extensions of the program for calculations of amorphous structures and structural relaxations.

[1] A. Thiess et al., *Phys. Rev. B* 85, 235103 (2012).

MM 10.3 Mon 12:15 IFW D

Large scale supercell calculations for forces around substitutional defects in NiTi — ●RUDOLF ZELLER — IAS-3, Forschungszentrum Jülich GmbH

Density functional calculations are used to investigate the force field arising from substitutional Ni and Cu defect atoms on Ti sites in the shape memory alloy NiTi. The forces for the unrelaxed atomic positions are calculated by the Korringa-Kohn-Rostoker (KKR) Green-function method for the experimentally found monoclinic B19' ground state structure. The force pattern in the vicinity of the defect atoms is markedly different between 32-atom and 256-atom supercells while it is nearly the same between 256-atom and 2048-atom supercells. This difference is explained by symmetry arguments and its possible implication on the concentration dependence of the transition from the high temperature B2 phase to the low temperature B19' or strain glass

phases is discussed.

MM 10.4 Mon 12:30 IFW D

Analytic Bond-Order Potential for Fe and Fe-C — ●SEBASTIAN SCHREIBER, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — Ruhr-Universität Bochum, Universitätsstr. 150, 44801 Bochum

The analytic bond-order potential (BOP) is an interatomic potential, that provides a linear scaling solution to the tight-binding (TB) energy. It includes itinerant magnetism and charge transfer explicitly and may be viewed as a systematic extension of second-moment models (e.g. Finnis-Sinclair) to include higher moment contributions. In the analytic BOPs the bond-order, the density of states, the atomic magnetic moments and charges adjust self-consistently according to the atomic environment. The analytic BOP also provides exact derivatives of the energy for calculating forces and stress.

Here, we demonstrate the transferability of recently developed TB models for Fe and Fe-C to the analytic BOP formalism. We present BOP simulations for core structures and Peierls barriers of a/2[111]-screw-dislocations in α -Fe. We also discuss the interaction of these line-defects with carbon impurity atoms and its impact on plastic deformation.

MM 10.5 Mon 12:45 IFW D

Efficient implementation of analytic bond-order potentials — ●THOMAS HAMMERSCHMIDT¹, SEBASTIAN SCHREIBER¹, BERNHARD SEISER², MICHAEL FORD², DAVID PETTIFOR², and RALF DRAUTZ¹ — ¹ICAMS, Ruhr-Universität Bochum, Germany — ²MML, University of Oxford, United Kingdom

The bond-order potentials (BOPs) are based on tight-binding (TB) models that are derived from density-functional theory. The BOPs provide an approximation to the TB energy that can be systematically improved by increasing the number of moments considered in the expansion. At the lowest level of two moments, the BOPs are equivalent to the Finnis-Sinclair potential and the closely related embedded-atom method. By taking into account higher moment contributions a systematic convergence to the TB energy is observed. We present an efficient implementation of analytic BOPs in close connection to a review of the BOP methodology. We will particularly discuss the fast identification of self-returning hoppings paths, the linear-scaling implementation of analytic forces and the performance of different self-consistency schemes. We will present recent results for several materials to illustrate the application to large-scale simulations.

MM 10.6 Mon 13:00 IFW D

Self-energy electronic structure renormalization effects in first-principles calculations of solids — ●ALBERTO MARMODORO¹, ARTHUR ERNST¹, PAOLO TREVISANUTTO², and LEONID SANDRATSKII¹ — ¹Max-Planck-Institut für Mikrostrukturphysik, Halle — ²Istituto Italiano di Tecnologia, Lecce

We report on a first-principles KKR-DFT calculation scheme for the evaluation of finite relaxation time and general bands structure renormalization effects for electrons in a solid. These are expressed in terms of an ad-hoc self-energy term on top of a reference hamiltonian, to which higher order corrections may be added. The case of substitutional disorder represents a well-known possible mechanism that gives raise to such phenomenology, here further pursued in the particular direction of including low-lying excitations above the globally colinear magnetic ground state of a magnetic material.

MM 11: Microstructure and Phase Transformations II - Nucleation/Solidification

Time: Monday 11:30–13:00

Location: IFW B

MM 11.1 Mon 11:30 IFW B

Determination of nucleation rates in a miscibility gap — ●CHRISTIAN SIMON¹, YIKUN ZHANG^{1,2,3}, and GERHARD WILDE¹ — ¹Westfälische Wilhelms Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster — ²Key Laboratory of Electromagnetic Processing of Materials, Northeastern University, Shenyang 110004, China — ³Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51147 Köln

A wetting transition from partial wetting to complete wetting is possible in alloys with a liquid miscibility gap. At a temperature T_p below the critical temperature T_c the alloy separates in a two-phase liquid system which plays an essential role in the microstructure formation of monotectic alloys. One of the liquid phases covers completely the surface of the other phase and the container walls. After the solidification of the first phase, this phase may act as heterogeneous nucleation site for the second phase. We present data of the Bismuth-Gallium system that has a miscibility gap with a critical point at 70 at% Gallium. The aim of the present study is the analysis of the nucleation rate of the crystalline phases with and without a liquid phase separation. We use a self-designed fast scanning calorimeter (up to 10 000 K/s) with nanowatt resolution in order to measure a statistical relevant data set of nucleation temperatures. With the help of the fast scanning calorimeter, we are able to prevent long range phase separation by fast cooling. The nucleation rate is evaluated by a statistical analysis that treats nucleation as a non-homogenous Poisson process.

MM 11.2 Mon 11:45 IFW B

Dependence of accessible undercooling on prior liquid over-heating by differential fast scanning calorimeter — ●BIN YANG¹, JOHN H. PEREPEZKO², JÜRN W. P. SCHMELZER¹, YULAI GAO³, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Department of Materials Science and Engineering, University of Wisconsin-Madison, 1509 University Avenue, Madison, WI 53706, USA — ³School of Materials Science and Engineering, Shanghai University, Shanghai 200072, P.R. China

The dependence of accessible undercooling on prior overheating of a pure tin single micron-sized droplet was studied by differential fast scanning calorimetry (DFSC) with cooling rates from 500 to 10,000 K/s. It is observed experimentally that (i) the degree of undercooling increases first gradually with increasing of prior overheating and reaches then an undercooling plateau; (ii) the accessible undercooling increases initially with increasing cooling rate. However, above a certain cooling rate the accessible undercooling decreases strongly with increasing cooling rate. For overheating levels above that for the onset of the undercooling plateau the undercooling increases with increasing cooling rate. These observed unusual behavior is successfully explained by heterogeneous nucleation in cavities. This mechanism can possibly also describe nucleation in other similar rapid solidification processes.

MM 11.3 Mon 12:00 IFW B

Analysis of the size effect and interfacial structure on the solidification and melting behavior of embedded Bi nanoparticles — ●TAE EUN SONG, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of material physics, Wilhelm-Klemm-Strasse, D-48149, Münster, Germany

Abstract Bi nanoparticles embedded in Zn or Al matrices were synthesized by rapid solidification and casting. The kinetics of Bi nanoparticles solidification has been examined by heating and cooling experiments in a differential scanning calorimeter (DSC). Upon heating in the DSC two Bi melting signals occur, one close to the eutectic temperature and the other at a lower temperature. Subsequent cooling leads to two solidification signals. Some Bi particles solidify at a small undercooling with a sharp exothermic peak, whereas other Bi particles solidify at a larger undercooling with a broad exothermic peak. The microstructure was analyzed by transmission electron microscopy (TEM). Cast samples show embedded Bi particles with a size larger than 80 nm and melt spun samples show embedded Bi nanoparticles with a size larger than 5 nm. The Bi nanoparticles that have an elongated and faceted morphology show an orientation relationship with the matrix. The solidification is interpreted using the classical theory of heterogeneous nucleation. Analysis of the results emphasizes the

important role of the local microstructure of embedded Bi nanoparticles and of the liquid*solid interface of embedded Bi nanoparticles with matrix.

MM 11.4 Mon 12:15 IFW B

Dendritic growth of tenfold twins from an undercooled melt of NiZr — ●RAPHAEL KOBOLD^{1,2}, WOLFGANG HORNEFECK¹, MATTHIAS KOLBE¹, and DIETER HERLACH^{1,2} — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — ²Ruhr-Universität Bochum, 44780 Bochum, Germany

The solidification of the intermetallic, congruent melting binary alloy Ni50Zr50 is studied in a temperature regime between the melting and the glass transition temperature. This system is well known as a good glass former in a broad concentration range of 30 to 80 at.% Zr. It is studied as a glass forming material, but it has as well a rare behaviour in solidification. We use electrostatic levitation technique to melt and undercool samples with a diameter of 2-3 mm under ultra-high-vacuum conditions. Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures since heterogeneous nucleation on container walls is completely avoided. During crystallisation the rapid increase of the temperature at the solid-liquid interface makes the solidification front visible. The solidification front is recorded by using a high-speed camera with a frame rate of 10.000 (1024x744) frames per second. At high undercoolings the solidification front of Ni50Zr50 shows features which make the investigation of its solidification behaviour particularly interesting. We observed the growth of a solidification front with 10-fold symmetry at a high undercooling temperature of approximately 300 K and a cooling rate of 53 K/s. Funding by Deutsche Forschungsgemeinschaft, under grant HE1601/18.

MM 11.5 Mon 12:30 IFW B

Kristallisationsverhalten und Kompositionsbestimmung von GeSbTe auf Si(111) mittels in-situ Transmissionselektronenmikroskopie und Elektronenenergieverlustspektroskopie — ●KATJA HAGEMANN, XIANG KONG und ACHIM TRAMPERT — Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland

Die Funktionalität von Phasenwechselmaterialien wie Ge-Sb-Te-Verbindungen (GST) basiert auf einer schnellen und reversiblen Phasenumwandlung zwischen amorphem und kristallinem Zustand. An dieser Stelle wird zunächst der amorphe Ausgangszustand strukturell analysiert und beschrieben. Anschließend wird der Einfluss eines einkristallinen Si-Substrats auf das Kristallisationsverhalten mittels in-situ Transmissionselektronenmikroskopie (TEM) im Temperaturbereich von Raumtemperatur bis 600°C untersucht. Im Bereich der amorph-kristallinen Übergangstemperatur (120-140°C) wird ein homogenes Keimbildungsverhalten mit einem anschließenden lateralen Kornwachstum beobachtet. Oberhalb der zweiten Übergangstemperatur (400-600°C) konnte erstmals eine Umorientierung und Ausrichtung der Kristallstruktur bezüglich des Substrates beobachtet werden. Es werden zwei Mechanismen zur Ausbildung dieser Orientierung diskutiert. Für die eingehende Untersuchung ist eine exakte Bestimmung der chemischen Komposition insbesondere in Hinblick auf die Homogenität auf der Nanometer-Skala entscheidend. Die Bestimmung der chemischen Zusammensetzung des ternären GST erfolgte mittels Elektronenenergieverlustspektroskopie (EELS) sowohl am amorphen Ausgangszustand wie auch am kristallinen Endzustand.

MM 11.6 Mon 12:45 IFW B

Dendritic growth kinetics of undercooled Fe-B alloy melts — ●CHRISTIAN KARRASCH^{1,2}, THOMAS VOLKMANN¹, and DIETER HERLACH^{1,2} — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — ²Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum, Germany

In metallic alloys dendritic growth is the major crystal growth mode controlling the evolution of the microstructure during solidification. The present work investigates the growth kinetics on pure Fe and Fe-B alloy melts in order to verify models for dendritic growth in undercooled melts. In detail, we analyze the effect of solute redistribution and solute trapping on the rapid growth of dilute Fe-1 at.% B alloy with B showing a small partitioning coefficient. For in-situ studies on

deeply undercooled melts electromagnetic levitation technique (EML) is used. The rapid solidification is recorded by a high-speed camera. Undercoolings from 50 K to 300 K prior to solidification leads to growth velocities of several cm/s up to m/s. Concerning terrestrial EML the electromagnetic field necessary for levitation induces strong convective fluid flow inside the melt. To investigate the effect of convection on the

growth kinetics experiments on parabolic flight are carried out under reduced gravity conditions. The microstructure of the solidified sample is analyzed by SEM and EBSD. Experimental results will be presented and discussed in the frame of current models for dendritic growth in undercooled melts. This research work is supported by DFG contract HE1601/18 and by ESA under contract 4200020277 and 4200014980.

MM 12: Invited Talk (Hauptvortrag) Hart

Time: Monday 15:00–15:30

Location: BAR 205

Invited Talk MM 12.1 Mon 15:00 BAR 205
Building Thermodynamic Models Made Easy: A Bayesian Compressing Sensing Approach to Automatically Cluster-Expanding 1500 Alloy Systems — ●GUS L. W. HART¹, LANCE J. NELSON¹, CONRAD W. ROSENBROCK¹, FEI ZHOU², and VIDVUDS OZOLINS² — ¹Dept. of Physics and Astronomy, Brigham Young Univ., Provo UT 84602 USA — ²Dept of Mat. Sci. and Engineering, University of California, Los Angeles CA 90095 USA

When building physical models (truncated expansions, force-fields, etc.), one often employs the widely-accepted intuition that the physics is determined by a few dominant terms. This reductionist paradigm

is limited because the intuition for identifying the those terms often does not exist or is difficult to develop. A "Bayesian compressive sensing" technique provides simple, general, and computationally efficient solution to this challenge. Combined with the high-throughput first principles approach to materials, BCS makes it possible to automatically build models for binary alloy models without human monitoring. Furthermore, the method can automatically adjust to generate the simplest model (fewest terms) that meets a specific accuracy requirement. Beyond the alloy applications, our BCS code can readily be applied to other model building problems. One merely needs a basis representation and training data to build a model in just a few seconds.

MM 13: Topical Session: Nanomechanics of nanostructured materials and systems III - Small scale plasticity

Time: Monday 15:45–17:45

Location: BAR 205

Topical Talk MM 13.1 Mon 15:45 BAR 205
Elevated Temperature, In-situ Microcompression Methods — ●JOHANN MICHLER, REJIN RAGHAVAN, and JEFFREY WHEELER — EMPA, Thun, Switzerland

The small size of nano-mechanical testing equipment creates opportunities for incorporating the equipment into different micro-analysis instruments: SPM, SEM, EBSD, optical probes, etc. This allows in situ sample surface imaging and in-situ microstructure analysis during mechanical testing. In the first part of the talk, we will describe a general nano-mechanical test platform capable of performing variable temperature and variable strain rate testing of micropillars in situ in the scanning electron microscope. Stable, elevated temperature indentation/micro-compression requires the indenter tip and the sample to be in thermal equilibrium to prevent thermal displacement drift due to thermal expansion. This is achieved through independent heating and temperature monitoring of both the indenter tip and sample. Furthermore, the apex temperature of the indenter tip is calibrated, which allows it to act as a referenced surface temperature probe during contact. In the second part of the talk, several case studies based on elevated temperature microcompression experiments will be presented: shear band kinetics in amorphous metals, brittle ductile transitions in Silicon, GaAs, GaN and InSb micropillars, and mechanical behaviour of nanolaminates.

MM 13.2 Mon 16:15 BAR 205
Finite volume effects on dislocation organization and associated size effects in strength — ●ERICA LILLEODDEN and HENRY OVRI — Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

The nearly universal observation of size effects from nanoindentation and microcompression experiments in metals has led to heated debate regarding the physical basis of such behaviors. Much research in this area has focused on the scaling of stress with deformation length scale, and largely ignores the important observation of the inherently jerky load-displacement response common to both experiments. Borrowing ideas from self-organized criticality, it is argued here that consideration of the displacement bursts in relation to the deformation and microstructural length-scales can help provide a framework for understanding size effects in plasticity. The talk will focus on single crystalline high purity Mg and the Mg alloy AZ31 of two orientations associated with dislocation plasticity (i.e., no twinning), where the active slip systems for the two orientations have significantly different Peierls barriers. In this way, we are able to differentiate the influence

of intrinsic lattice strength and alloying content. It will be shown that the distribution of displacement bursts and their associated stresses can be used to investigate the combined influences of finite volumes and material & microstructural parameters on the organization of dislocation structure and resultant stress-strain response.

MM 13.3 Mon 16:30 BAR 205
Size-dependent plasticity in KCl and LiF single crystals: Influence of orientation, temperature, pre-straining and doping — ●YU ZOU and RALPH SPOLENAK — Laboratory for Nanometallurgy, Department of Materials, ETH Zurich, Zurich, Switzerland

Size dependence of plasticity is generally observed and intensively studied in metallic systems, but it is rarely investigated in ionic crystals. In this work, two typical ionic crystals with the rocksalt structure, KCl and LiF, were investigated using micro-compression technique. Single-crystalline KCl and LiF pillars with diameters ranging from four microns to two hundred nanometers were produced by focused ion beam milling. The pillars were compressed using a flat-punch tip in a nanoindenter, along [001]- and [111] orientations and at both room temperature and ~200 °C. Pre-strained [111] LiF and CaCl₂ doped [001] KCl pillars were compressed as well. We found that, in contrast to KCl, the size-dependence in LiF pillars is more sensitive to the orientation and temperature change. [111] LiF exhibit smaller size dependence and displacement bursts than the other pillars measured. The results also show that the pre-straining strengthens [111] LiF pillars in micron-sized range but weakens them in submicron-sized range, resulting a reduced size-effect exponent. The doping in [001] KCl slightly increases strength levels and decreases the size dependence. Generally, in terms of size-effect phenomenon, [111] LiF is similar as body-centered-cubic metals, while [001]- and [111] KCl and [001] LiF are comparable with face-centered-cubic metals. The additivity of strengthening mechanisms is critically discussed.

15 min break

MM 13.4 Mon 17:00 BAR 205
Influence of microalloying on the mechanical properties of molybdenum disilicide — ●CAROLIN PUSCHOLT¹, STEFFEN NEUMEIER¹, MATHIAS GÖKEN¹, and SANDRA KORTE-KERZEL² — ¹FAU Erlangen-Nürnberg, Germany — ²RWTH Aachen, Germany

Molybdenum disilicide (MoSi₂) is a very promising candidate material for high temperature structural applications due to its high melting point (2030°C), low density and good oxidation resistance. However,

the use of the pure material is limited by its low fracture toughness below 900°C which is associated with the plastic anisotropy and the high critical resolved shear stress on particular slip systems.

Microalloying of MoSi₂ clearly enhances the room temperature ductility. For example, Ta, Al and Nb increase the ductility due to the activation of an additional slip system. However, the underlying mechanisms by which ductility is improved remain poorly understood, predominantly due to the difficulties encountered in low temperature experiments along the most brittle crystal orientation [001].

Here, this problem is overcome by using characterization methods at the microscale. A combination of uniaxial testing, where cracking is suppressed and hence the critical resolved shear stresses in specific crystal orientations can be determined individually, and nanoindentation in conjunction with EBSD and TEM was used. Results on pure and microalloyed MoSi₂ with Tantalum will be presented, focusing on the influence of microalloying on the critical resolved shear stresses of particular slip systems.

MM 13.5 Mon 17:15 BAR 205

On The Importance Of Twinning Wedges in Nanowhisker Bending — JOHANNES J. MÖLLER, WOLFRAM NÖHRING, and •ERIK BITZEK — Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Single crystalline metallic nanowhiskers have attracted substantial interest due to their special mechanical behavior. Similar to other nanostructured metals, like nano-pillars, thin films and nanocrystalline samples, they show a pronounced "smaller is stronger"-effect. However, not only the strength but also the deformation mechanisms can be size-dependent. Recently, twinning has been observed to be the governing deformation mechanism of <110>-oriented gold nanowhiskers under tension, whereas under compression they deform by nucleation and glide of full dislocations. Here, we address the question how nanowhiskers deform under bending loads. For this purpose we performed atomistic simulations of Au, Cu and Mo nanowhiskers using

set-ups modeling three-point bending and the bending of a clamped cantilever beam. Independent on temperature, deformation rate, size and aspect ratio, the occurrence of wedge-shaped twins in the tensile region of the bent whisker was a characteristic feature in all simulations. Whereas the tendency for twinning can be explained by analyzing the generalized stacking fault energy and the resolved shear stresses on the partial dislocations, the particular wedge shape of the twins can be directly rationalized by the strain gradient within the bent whiskers.

MM 13.6 Mon 17:30 BAR 205

Mechanical stability of quasi one-dimensional nanostructures (nanowires) — •CHARLOTTE ENSSLEN, OLIVER KRAFT, and REINER MÖNIG — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Nanostructured materials are of interest for both fundamental scientific and applied research which can be ascribed to their outstanding mechanical properties, e.g. Au nanowires can exhibit high strength and ductility. In general, it can be observed that a decrease in the sample dimension results in an increase in strength known as mechanical size effect. However, data considering the mechanical properties of nanostructures with dimensions smaller than 100 nm are still rare and the corresponding deformation mechanisms and the interrelations of the microstructure, e.g. the role of inherent defects, have not been fully understood. In order to develop a profound understanding of the role of defects for the deformation mechanisms of single- and polycrystalline nanowires we make use of a helium ion microscope. It offers the possibility to design and modify nanostructures, altering the surface characteristics or creating nanopores in the nanowire prior to mechanical testing. The stress-strain curves and the deformation mechanisms of pristine and modified Au and Si nanowires are presented as recent examples. Whereas modified Si nanowires show a decreased tensile strength and a brittle failure at the defects, the mechanical behavior of modified Au nanowires seems to be independent of the defects.

MM 14: Functional Materials III - Li ion batteries

Time: Monday 15:45–17:15

Location: IFW A

MM 14.1 Mon 15:45 IFW A

Studying the phase growth in LFP thin films — •FABIAN WUNDE¹, FRANK BERKEMEIER¹, and GUIDO SCHMITZ² — ¹Institut für Materialphysik Universität Münster — ²Institut für Materialwissenschaft Universität Stuttgart

Lithium Iron Phosphate (LFP) is one of the state of the art cathode materials for lithium ion batteries. In this work, LFP thin films between 100 and 300 nm are deposited by ion beam sputtering. These films exhibit a reasonable electrochemical capacity and excellent cycle life stability, which makes them capable for fundamental research, like diffusion studies. Therefore, detailed cyclic voltammetry (CV) measurements are carried out on the films. According to Randles and Sevcik, the peak current of the CV diagrams is found to be proportional to the squareroot of the scan rate, but studies on LFP films of different thickness also show a proportionality to the film thickness. The latter differs from the theory of Randles and Sevcik and is expected to be due to the two-phase nature of LFP, forming a lithium-rich and a lithium-poor phase. Therefore, we numerically study the growth and descent of the two phases, by means of finite differences methods, using a discrete diffusion model and chemical potentials obtained from the regular solution. Within these studies, the time-dependence of the lithium content of the LFP is evaluated, and correlated to the experimental data.

MM 14.2 Mon 16:00 IFW A

The electrocapillary coupling in aprotic lithium electrolytes — •TOBIAS KITZLER¹, JÜRGEN MARKMANN^{1,2}, and JÖRG WEISSMÜLLER^{1,2} — ¹Helmholtz-Zentrum Geesthacht — ²Technische Universität Hamburg-Harburg

During lithium loading and unloading into metal anodes, the electrodes undergo considerable volume change. Whenever there are gradients in composition, the volume change is accompanied by large internal stress. Depending on the mechanism of solution of Li into the electrode material, this results in different values for the electrocapillary coupling parameter (ECCP), which is here a change of apparent sur-

face stress with apparent surface charge density and can be measured using the identity with change of electrode potential with elastic strain. Therefore the potential dependent ECCP can be used to analyse the Lithium solution mechanisms. In this talk, we present experimental results for the ECCP of a thin film gold electrode which was measured from the potential modulation when the electrode was cyclically strained in-situ during lithiation. We show supporting in-situ x-ray lattice parameter data, also measured on the films in-situ during lithiation. The underlying microscopic processes are discussed in relation to the observed ECCP.

MM 14.3 Mon 16:15 IFW A

All solid-state batteries using lithium iron phosphate and tin as electrodes — •SUSANN NOWAK¹, FRANK BERKEMEIER², and GUIDO SCHMITZ¹ — ¹Institut für Materialwissenschaften, Heisenbergstr. 3, 70569 Stuttgart — ²Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Thin-film all solid-state batteries have been prepared using lithium iron phosphate (LFP) as the cathode, lithium phosphoroxide oxynitride (LiPON) as a solid-state electrolyte, and tin as an anode. All layer preparations are carried out using ion beam sputtering which yields a battery of below 1 μm thickness on oxidized silicon. These all solid-state battery is characterized by means of electrochemical properties using chronopotentiometry (CP) and electrochemical impedance spectroscopy (EIS). Additionally the micro structure of the cells is investigated by transmission electron microscopy (TEM) and electron diffraction. It is found that in comparison to a system in liquid electrolyte (lithium perchlorate in EC/DEC) the all solid-state system gives very similar results and therefore presents an interesting and suitable model system for further studies of the behavior of lithium ion batteries, for example the investigation of the behavior at higher temperatures than possible in case of a liquid electrolyte.

MM 14.4 Mon 16:30 IFW A

Diffusion and Interface Transport in LCO Thin-Films — •FRANK BERKEMEIER, TOBIAS STOCKHOFF, and GUIDO SCHMITZ —

Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Lithium cobalt oxide (LCO) thin-films are prepared by ion-beam sputter deposition. The capability of the films to reversibly store and release lithium ions is proven by cyclic voltammetry and chronopotentiometry. It is demonstrated that the lithium concentration of the films can be reliably determined by electrochromic absorption technique using visible light, which even allows to measure the time-dependence of the lithiation/delithiation reaction. Using this electrochromic absorption technique, the intercalation of lithium into LCO is studied in case of films between 10 and 400 nm in thickness. To describe the intercalation reaction in a proper way, it is found that – apart from the volume diffusion – the interface transport of lithium has to be taken into account. Therefore, we suggest a diffusion model which includes an interface transport coefficient that considers the transfer of lithium ions from the liquid electrolyte into the LCO. Using this model, we are able to accurately describe the experimental data, and determine the interface transport coefficient to $\approx 10^{-7}$ cm/s.

MM 14.5 Mon 16:45 IFW A

Functional Thin-Films for Li-Ion Batteries Grown by Novel CO₂-Laser Assisted Chemical Vapor Deposition — ●CHRISTOPH LOHO¹, AZAD DARBANDI^{1,2}, RUZICA DJENADIC^{1,3}, OLIVER CLEMENS^{1,2}, and HORST HAHN^{1,2,3} — ¹Joint Research Laboratory Nanomaterials, Technical University of Darmstadt and Karlsruhe Institute of Technology, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — ³Helmholtz 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, en-

ergy 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.

We report on the functional thin-film synthesis via CO₂-laser assisted chemical vapor deposition (LACVD). The use of a CO₂-laser as part of the precursor delivery system is unique in the field of thin-film deposition so far and thus will be introduced. Furthermore, the characterization of a cathode (LiCoO₂) as well as solid-state electrolyte (Li₇La₃Zr₂O₁₂) material for thin-film Li-ion batteries is presented. In addition to results on the microstructure and composition of these materials we give an account of their electrochemical performance.

MM 14.6 Mon 17:00 IFW A

Effect of Ni-doping on structural, magnetic and electrochemical properties of LiMn_{1-x}Ni_xPO₄ — ●ALEXANDER OTTMANN¹, CARSTEN JÄHNE¹, HANS-PETER MEYER², and RÜDIGER KLINGELER¹ — ¹Kirchhoff-Institute for Physics, University of Heidelberg, Germany — ²Institute of Earth Sciences, University of Heidelberg, Germany

Nanoscaled polycrystalline LiMn_{1-x}Ni_xPO₄ with a doping level of x up to 0.45 has been synthesized via a microwave-assisted hydrothermal route. Characterization of the materials by means of X-ray powder diffraction, scanning electron microscopy, energy dispersive X-ray spectroscopy and SQUID-magnetometry confirm well controlled Ni-doping in LiMnPO₄. The data show solid solution behaviour with the lattice parameters linearly decreasing upon increasing the nickel concentration, corresponding to Vegard's law. Concomitantly, the room temperature magnetization decreases which implies substitution of Mn²⁺ by Ni²⁺ in the LiMnPO₄ host structure. Electrochemical characterization by means of cyclic voltammetry reveals an active Mn³⁺/Mn²⁺ redox couple. The redox potential depends on the nickel concentration in LiMn_{1-x}Ni_xPO₄ and increases with x . Quantitatively, the reduction potential vs. lithium increases from 3.97 V in LiMnPO₄ to 4.09 V in LiMn_{0.55}Ni_{0.45}PO₄.

MM 15: Computational Materials Modelling III - Bulk thermodynamics/ Phase Transitions I

Time: Monday 15:45–17:45

Location: IFW D

MM 15.1 Mon 15:45 IFW D

Impact of weak and strong magnetic coupling on the thermodynamics of chromium — ●FRITZ KÖRMANN, BLAZEJ GRABOWSKI, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

Chromium is a decisive ingredient for stainless steels and a reliable understanding of its thermodynamic properties is thus indispensable. Parameter-free first-principles methods have nowadays evolved to a state allowing such thermodynamic predictions. For materials such as Cr, however, the inclusion of magnetic entropy and higher order contributions such as anharmonic entropy is still a formidable task. Employing state-of-the-art ab initio molecular dynamics simulations and statistical concepts, we compute a set of thermodynamic properties based on quasiharmonic, anharmonic, electronic and magnetic free energy contributions from first principles [1]. The magnetic contribution is modeled by an effective nearest-neighbor Heisenberg model, which itself is solved numerically exactly by means of a quantum Monte Carlo method. We investigate two different scenarios: a weak magnetic coupling scenario for Cr, as usually presumed in empirical thermodynamic models, turns out to be in clear disagreement with experimental observations. We show that only a mixed Hamiltonian including weak and strong magnetic coupling provides a consistent picture with good agreement to experimental thermodynamic data.

[1] F Körmann, B Grabowski, P Söderlind, M Palumbo, S G Fries, T Hickel and J Neugebauer, *J. Phys.: Condens. Matter* 25, 425401 (2013).

MM 15.2 Mon 16:00 IFW D

Thermomechanical properties of α -iron from first-principles — ●DANIELE DRAGONI¹, DAVIDE CERESOLI², and NICOLA MARZARI¹ — ¹THEOS - École Polytechnique Fédérale, Lausanne, Switzerland — ²ISTM - Istituto Nazionale delle Ricerche, Milano, Italy

Compliance tensors provide a full characterization of the mechanical response of crystals in the linear regime of stress-strain. Their prediction from first-principles is of great practical utility, given the large number of elastic constants that are not known experimentally, while also pro-

viding stringent tests for validation of electronic-structure approaches in those cases where accurate experimental numbers are available. Since the intrinsic temperature dependence of the elastic constants is determined by the vibrations of the crystal (a Bose-Einstein gas of harmonic oscillators), finite-temperature results can be computed, in the quasiharmonic approximation, from the equation of state for the materials at hand and the volume- or strain-dependence of the phonon frequencies. We use ferromagnetic bcc α -iron as a case study, carefully testing pseudopotential calculations against reference all-electron results at 0K, and cubic elastic constants at finite temperatures against experimental results.

MM 15.3 Mon 16:15 IFW D

Influence of magnetism on the stability of binary transition-metal compounds — ●ALVIN NOE LADINES, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — ICAMS, Ruhr Universität Bochum, Germany

Refractory elements (RE) play an important role in the development of creep-resistant ferritic steels for high temperature applications. They can act as solid solution strengthener or carbide-former but also lead to the precipitation of topologically close-packed (TCP) phases that may initiate embrittlement and fracture. It is thus important to predict the formation of TCP phases in multi-component alloys. An attempt to address this is the development of structure maps which relate the alloy stability to atomic-size difference and average band-filling of the constituents. In this study we quantify the influence of magnetism for a recently developed structure map for TCP phases of transition-metal compounds. Based on density functional theory (DFT) calculations of the heat-of-formation of TCP phases in several Fe-RE systems over the whole range of chemical composition, we derive a model that correlates the magnetic energy to the average band filling of the compounds. This can be understood within the Stoner model of itinerant magnetism where the magnetic moment on the atom corresponds to a rigid shift in the spin-polarized density of states. We rescale the structure map with respect to this shift.

MM 15.4 Mon 16:30 IFW D

Thermally stable h.c.p.-based phases in Ni-W thin films — ●SASCHA B. MAISEL¹, SILKE J. B. KURZ², ANDREAS LEINEWEBER², STEFAN MÜLLER¹, and ERIC J. MITTEMEIJER^{2,3} — ¹Institute of Advanced Ceramics, TUHH, 21073 Hamburg, Germany — ²Max Planck Institute for Intelligent Systems (formerly Max Planck Institute for Metals Research), 70569 Stuttgart, Germany — ³Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

In this combined experimental and DFT-based study, we demonstrate that even though the Ni-W phase diagram shows no h.c.p.-based phases, h.c.p.-like stacking sequences can be observed in magnetron-co-sputtered Ni-W thin films at W contents of 20 at.% to 25 at.%. The occurrence of these h.c.p. domains is rationalized from first-principles calculations, showing that the vicinity of the system's ground-state line is indeed populated with metastable h.c.p.-based structures in the intermediate concentration range from 20 to 50 at.%. The h.c.p.-like stacking in Ni-W is found to be thermally stable by performing extensive XRD analysis on samples before and after heat treatments up to 850 K.

15 min break

MM 15.5 Mon 17:00 IFW D

Ab initio based insights into structural transformations and the role of interfaces in Fe-C alloys — ●XIE ZHANG^{1,2}, TILMANN HICKEL¹, JÖRG NEUGEBAUER¹, JUTTA ROGAL², and RALF DRAUTZ² — ¹Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — ²Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität-Bochum, 44780 Bochum, Germany

Structural transformations in Fe-C alloys are decisive for the mechanical properties of various steels. We have combined first principles and the Solid State Nudged Elastic Band method to study the structural transformations in the Fe-C system and the role of interfaces in these processes. Our investigations revealed the occurrence of an intermediate structure, which can perfectly bridge austenite, ferrite and cementite. The formation of such a structure was found to be the result of an interfacial adaptive behavior to accommodate the misfit of lattice constants and the different magnetic states in both phases. These insights provide a detailed understanding on the origin of the complex structure of cementite and the formation mechanisms of com-

plex microstructures such as pearlite and bainite in steels.

MM 15.6 Mon 17:15 IFW D

Atomistic simulation of transformations at disordered FeCr bcc- σ interfaces — ●THOMAS SCHABLITZKI, JUTTA ROGAL, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

We study the transformation of the σ phase in FeCr to the bcc structure. We observe disordered interface region that have a thickness of several atomic layers. Transformation paths from one crystal phase to another get obfuscated by seemingly random movements and rearrangements in the interface and create a challenge to study the transformation processes, as well as increase the computational effort of the simulation. Using coordination polyhedra and topological fingerprints we look for correlations in processes in the interface region of FeCr bcc- σ interfaces and along transformation paths trying to identify the characteristic processes responsible for the phase transition.

MM 15.7 Mon 17:30 IFW D

First-principles approach to investigate hydrogen cluster formation in austenitic Mn-rich steels — ●AURAB CHAKRABARTY, ROBERT SPATSCHKE, TILMANN HICKEL, and JOERG NEUGEBAUER — Max-Planck Institute for Iron Research, Dusseldorf, Germany

Hydrogen related failure is a well-known problem in high-strength austenitic steels for automotive applications. Experiments provide evidences of reduced ductility and H-induced local plasticity (HELP) upon H charging in these materials. The HELP model provides an explanation for the formation and propagation of cracks in austenitic steel. An important criterion for HELP is segregation of hydrogen to topological defects such as stacking faults and grain boundaries and the mechanism of H-segregation in high-Mn steels is not completely understood yet. We used density functional theory (DFT) total energy calculation to estimate the interactions between H-interstitial atoms in Fe-Mn alloys and the influence of H on stacking faults. We observed enhanced H-H interaction in a hydrogen cluster, i.e. a local hydride phase. Furthermore, a lower solution energy provided by the presence of a stacking fault makes it a favourable site for H-accumulation. The interaction energies and elastic constants calculated using DFT are used in finite-temperature Monte-Carlo and continuum-scale analysis in order to predict a phase-diagram for a temperature driven phase separation of Fe into a dilute and a local hydride phase.

MM 16: Microstructure and Phase Transformations III - Precipitation hardening/ Alloying elements

Time: Monday 15:45–17:15

Location: IFW B

MM 16.1 Mon 15:45 IFW B

Atom Probe Tomography Analyses of Precipitation in the AA2195 Aluminum Lithium Alloy — ●MUNA KHUSHAIM¹, TORBEN BOLL¹, FERDINAND HAIDER², and TALAAT AL-KASSAB¹ — ¹King Abdullah University of Science and Technology (KAUST), Division of Physical Sciences and Engineering, Thuwal 23955-6900. Saudi Arabia — ²University Augsburg, Inst. f. Physik, D-86159 Augsburg, Germany

One of the primary materials used for structural components of aircrafts are aluminum-lithium alloys. These alloys exhibit an enhanced strength-weight ratio which makes them an attractive material for weight critical applications. This study focuses on the alloy 2195 (a member of a series of high strength Al-Li-Cu alloys known as Weldalite), which owes its superior mechanical properties to a thermo-mechanical treatment termed T8. The presence of different micro-alloying elements and an adequate heat treatment causes the precipitation of different phases such as T_1 (Al_2CuLi), θ' (Al_2Cu) and β' (Al_3Zr). Utilizing the laser assisted wide angle tomographic atom probe (LAWATAP) and local electrode atom probe (LEAP) allowed the characterization of the different precipitates that dominate the microstructure of this functional material and identify their role in the hardening process. Additionally, the effect of the microstructure on the mechanical properties of the alloy was estimated by measuring its micro-hardness.

MM 16.2 Mon 16:00 IFW B

Analysis of The Melting Process of Indium Nanoparticles Embedded in An Aluminium Matrix — ●MOSTAFA MOHAMED,

MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, Münster, Germany

We have successfully prepared nanocrystalline particles Indium embedded in an Aluminum matrix by rapid quenching using the melt-spinning technique. The microstructures and the melting temperature and freezing of the embedded nanoparticles were investigated by transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). The microstructure analysis exhibited two distributions of (In) particles embedded in the Al-matrix, one at the grain boundaries and the other within the Al matrix. DSC experiments have shown broad melting and crystallization peaks. The crystallization temperature of the embedded particles shifted to remarkable low temperature. Analyses of TEM images and DSC measurements were done to investigate the impact of the particle-matrix interface and interface modifications on the melting behavior of the embedded nanoparticles.

MM 16.3 Mon 16:15 IFW B

Phase transformation in Nb-H thin film — ●VLADIMIR BURLAKA, STEFAN WAGNER, and ASTRID PUNDT — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Physical properties of nano-sized metal hydrogen systems strongly change with mechanical stress, evolving during hydrogen loading and phase transition. For very thin films stress relaxation processes are expected to be much less efficient compared to thick films. Thus the systems will stay in a high-stress state. This changes the system's thermodynamics and kinetics [1,2].

In this in-situ STM study we use epitaxial Nb-H thin films of thick-

nesses with less than 50nm as a model system. By performing constant pressure hydrogen loading sequences on films of different thickness we address differences in hydride precipitation and growth during the phase transformation. To approve and study the role of mechanical stresses conservation, the in-situ STM results are completed by in-situ XRD results providing a macroscopic overview of the sample's lattice structure during the hydrogen uptake.

Financial support by the DFG via project PU131/12-1 is gratefully acknowledged. Beamtime is kindly provided by the DESY, at PETRA beamline P08.

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

MM 16.4 Mon 16:30 IFW B

Neue massive beta-Ti-Nb-In Legierungen für Knochenimplantatanwendungen — ●ARNE HELTH^{1,2}, STEFAN PILZ^{1,2}, MARIANA CALIN¹, ANNETT GEBERT¹ und JÜRGEN ECKERT^{1,2} — ¹Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — ²Institut für Werkstoffwissenschaft, TU Dresden

Der zunehmende Einsatz Ti-basierter Werkstoffe für nicht-degradable Knochenimplantate erfordert eine ständige Weiterentwicklung der biofunktionellen Werkstoffeigenschaften. Hierbei liegt der Fokus zum einen auf der Einstellung einer hohen Dauerfestigkeit, zur Verhinderung von Ermüdungsfrakturen und zum anderen auf der Anpassung der elastischen Eigenschaften an die des kortikalen Knochens, um *stress shielding* zu vermeiden.

Ausgangspunkt der vorliegenden Arbeit ist die binäre beta-Ti-Legierung Ti-40Nb. Sie weist neben einer exzellenten Korrosionsbeständigkeit Druckfestigkeiten von bis zu 1400 MPa und einen E-Modul von ~60 GPa auf. Ziel war es, durch die Zulegierung von Indium den E-Modul weiter abzusenken. Durch eine thermomechanische Behandlung sollen die mechanischen Eigenschaften im Sinne der Biofunktionalität optimiert werden.

Durch die Addition von 5 m.% Indium konnte ein minimaler E-Modul von 49 GPa erreicht werden. Im Rahmen der thermomechanischen Prozessierung wurde die mittlere Korngröße maßgeblich abgesenkt und eine Festigkeitssteigerung von über 10 % im Vergleich zum Gusszustand erreicht. Durch eine anschließende Stufenglühung konnten Festigkeit von über 550 MPa eingestellt werden.

MM 16.5 Mon 16:45 IFW B

Phase transformations in Ti-Fe and Ti-Fe-Nb alloys by in situ X-ray diffraction — ●OLGA SHULESHOVA¹, IVAN KABAN^{1,2}, DIRK HOLLAND-MORITZ³, JAN GEGNER³, FAN YANG³, JOZEF BEDNARCIK⁴, JUNHEE HAN¹, NORBERT MATTERN¹, and JÜRGEN ECKERT^{1,2} — ¹IFW Dresden, Institute for Complex Materials, 01171 Dresden, Germany — ²TU Dresden, Institute of Materials Science, 01062 Dresden, Germany

MM 17: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II (O with HL/TT/MM)

Time: Monday 16:00–18:45

Location: TRE Ma

Topical Talk MM 17.1 Mon 16:00 TRE Ma
Simulating heat transport: from large scale molecular dynamics to first-principles calculations — ●DAVIDE DONADIO — Max Planck Institute for Polymer Research, Mainz, Germany

The necessity to design materials and devices able to harness thermal energy, and possibly convert it into more amenable energy forms, has stimulated a major effort in the scientific community to understand heat transport at the mesoscale and the nanoscale. In this talk I will discuss different atomistic approaches to simulate nanoscale heat transport, ranging from large scale molecular dynamics simulations with classical empirical potentials at equilibrium and non-equilibrium conditions, to lattice dynamics calculations with force-constants computed by first principles. Applications will include silicon and carbon nanostructures, phase-change materials and molecular junctions.

MM 17.2 Mon 16:30 TRE Ma

First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides — ●ANKITA KATRE¹, ATSUSHI TOGO², RALF DRAUTZ¹, and GEORG K. H. MADSEN¹ — ¹ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — ²ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

— ³DLR, Institut für Materialphysik im Weltraum, 51170 Köln, Germany — ⁴DESY Photon Science, 22607 Hamburg, Germany

In this work the solid-liquid phase transformations, as well as phase equilibria in the binary Ti-Fe and ternary Ti-Fe-Nb systems are studied by means of in situ X-ray diffraction of the synchrotron radiation. To avoid contamination the reactive titanium alloys have been processed containerlessly, using electrostatic levitator. Levitated samples were repeatedly heated from the room temperature above their liquidus temperatures and subsequently cooled down to undergo solidification. Analysis of the lattice constants shows that below approx. 800°C solid-state diffusion is negligible and samples are only subjected to thermal expansion. On heating above this temperature near-equilibrium conditions are reached before the onset of melting. These data have been used to verify the binary Ti-Fe phase diagram and to map solidus and liquidus surfaces in Ti-rich corner of the ternary Ti-Fe-Nb system. On cooling the liquid melts were subjected to considerable undercooling. Detailed evolution of the lattice parameters of the samples solidified under non-equilibrium conditions is presented. Financial support by DFG under project No. SH 578/1-1 is gratefully acknowledged.

MM 16.6 Mon 17:00 IFW B

Droplet size distribution in liquid phase separated Cu75Co25-xMx (M = Fe, Ni) alloys with low M content — ●YIKUN ZHANG^{1,2}, ZHIKANG WU¹, MEIMEI WANG¹, JIANRONG GAO¹, CHAO YANG¹, and GERHARD WILDE² — ¹Key Laboratory of Electromagnetic Processing of Materials (Ministry of Education), Northeastern University, Shenyang 110004, China — ²Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Straße 10, D-48149 Münster, Germany

Liquid phase separation in metallic alloys has been investigated over the past sixty years. One of the most intensively studied systems is the binary Cu-Co system, which is a simple peritectic system, but has a metastable miscibility gap in the undercooled region because of a positive heat of mixing. A recent study indicated that a Zr addition can modify the surface energies and/or the wetting behavior in a peculiar way in the ternary Co-Cu-Zr system at low Zr content. In the present work, the effect of small amounts of an Fe/Ni addition on the liquid phase separation behavior in undercooled Cu75Co25-xMx (M = Fe, Ni and x = 1, 5) alloys has been studied by using the glass fluxing method. All the samples show a bimodal droplet size distribution, the center of the first peak position shifts to a larger radius gradually with increasing undercooling in Cu75Co24Ni. The Fe addition can promote the liquid phase separation behavior, but in contrast the Ni addition can suppress it effectively. The present results may provide valuable information for understanding the microstructure evolution in undercooled Cu-Co alloys.

Nano-structured Zinc-Chalcogenides are interesting for thermoelectric applications due to their low thermal conductivity.[1] A simple model study has reported how the thermal conductivity of ZnS, ZnSe and ZnTe can potentially show a cross-over as a function of the maximal mean free path of the phonons.[2] We have applied the Boltzmann transport equation in the relaxation time approximation to verify this. We find that thermal conductivity of ZnS crosses ZnSe and ZnTe and explain this in terms of the different contributions of phonon modes in these materials. Furthermore, the cross-over is found to be strongly influenced by isotope scattering. The calculated thermal conductivity is found to be strongly dependent on the volume and we explain the observed differences between LDA and GGA calculations. We compare further calculated thermal properties, such as the thermal expansion coefficient, to experiment to validate our approach.

[1] L.Zhen, S.Qiao, D.Y.Xiang, H.Z.Zhong, and Q.L.Gao, J. Mater. Chem. 22, 22821 (2012). [2] N.Mingo and D.Broido, Phys. Rev. Lett. 93, 246106 (2004).

MM 17.3 Mon 16:45 TRE Ma

Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals — ●HONGHUI SHANG, CHRISTIAN CARBOGNO, PATRICK RINKE, and MATTHIAS SCHEFFLER —

Fritz-Haber-Institut der MPG, Berlin

The response of the electronic structure to atomic displacements gives rise to a variety of interesting physical phenomena, which can be probed by experimental techniques such as infrared or Raman spectroscopy or neutron diffraction. The response can be conveniently computed from first principles by means of density-functional perturbation theory (DFPT). Here we present our implementation in the all-electron atom-centered numeric orbital code FHI-aims [1]. Our approach combines the accuracy of an all-electron full-potential treatment with the computational efficiency of localized atom-centered basis sets that is necessary to study large and complex systems. We verified the accuracy of our DFPT implementation by comparing the vibrational frequencies to finite-difference reference calculations and literature values. Due to the atom-centered nature of the integration grids in FHI-aims, the portion of the grid that belongs to a certain atom also moves when this atom is displaced. Here we demonstrate that, unlike for first derivatives (i.e. forces) [2], this moving-grid-effect plays an important role for second derivatives (i.e. vibrational frequencies). Further analysis reveals that predominantly diagonal force constant terms are affected, which can be bypassed efficiently by invoking translational symmetry.

[1] V. Blum et al. *Comp. Phys. Comm.* **180**, 2175 (2009)

[2] B. Delley, *J. Chem. Phys.* **94**, 7245 (1991).

MM 17.4 Mon 17:00 TRE Ma

Breakdown of Fourier law in layered materials — ●ANDREA CEPPELOTTI¹, GIORGIA FUGALLO², FRANCESCO MAURI³, and NICOLA MARZARI¹ — ¹THEOS, École Polytechnique Fédérale, Lausanne — ²IMPMC, Université Pierre et Marie Curie, Paris — ³LSI, École Polytechnique, Paris

We compute the thermal conductivity in crystalline layered materials by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. We find that in 2D materials, such as graphene and related compounds, and even in 3D layered materials, like bulk graphite, the single-mode relaxation time approximation (SMRTA) cannot describe heat transport correctly, underestimating by one order of magnitude or more thermal conductivities and phonons' mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in excellent agreement with experimental measurements [2]. The shortcomings of the SMRTA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations is often comparable with that of the experimental sample - as a result, Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths.

[1] G. Fugallo et al., *Phys. Rev. B*, **88**, 045430 (2013).

[2] A. A. Balandin, *Nat. Mater.* **10**, 569 (2011).

MM 17.5 Mon 17:15 TRE Ma

High Temperature Thermal Conductivity from First Principles — ●CHRISTIAN CARBOGNO¹, RAMPI RAMPRASAD², and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — ²Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, Boltzmann transport techniques [1] that include anharmonic effects only perturbatively become inaccurate or even inapplicable. In this work, we overcome this limitation by performing first-principles Green-Kubo simulations [2], in which all orders of anharmonicity are incorporated by the means of *ab initio* molecular dynamics. The thermal conductivity is then assessed from the auto-correlation function of the heat flux in thermodynamic equilibrium. We discuss the details of our implementation and the definition of our heat flux that is based on the virial theorem. We validate our approach by presenting calculations for ZrO₂ that also showcase the importance of higher order anharmonic effects in materials with low thermal conductivities. Eventually, we discuss how our technique can be coupled to multi-scale models to achieve a computationally efficient and accurate description of the thermal conductivity at the nanoscale.

[1] D. A. Broido et al., *Appl. Phys. Lett.* **91**, 231922 (2007).

[2] R. Kubo, M. Yokota, S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

MM 17.6 Mon 17:30 TRE Ma

Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles — ●ANTHONY REILLY and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

Molecular materials are of great fundamental and applied importance in science and industry, with numerous applications in pharmaceuticals, electronics, sensing, and catalysis. A key challenge for theory has been the prediction of their stability, polymorphism and response to perturbations. While pairwise models of van der Waals (vdW) interactions have improved the ability of density functional theory (DFT) to model these systems, quantitative and even qualitative failures often remain. Here, we show how a many-body description of vdW interactions can dramatically improve the accuracy of DFT for molecular materials, yielding quantitative description of stabilities and polymorphism for these challenging systems. Moreover, the role of many-body vdW interactions goes beyond stabilities to response properties. In particular, we have studied the elastic properties of a series of molecular crystals, finding that many-body vdW interactions can account for up to 30% of the elastic response, leading to quantitative and qualitative changes in elastic behavior. We will illustrate these crucial effects with the challenging case of the polymorphs of aspirin, leading to a better understanding of the conflicting experimental and theoretical studies of this system.

MM 17.7 Mon 17:45 TRE Ma

Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT? — ●DANIEL BERGER, HARALD OBERHOFER, and KARSTEN REUTER — Technische Universität München, Germany

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. For first-principles modeling of corresponding surface chemical reactions the current state-of-the-art is generally defined by hybrid-level density-functional theory (DFT). Systematic work assessing the achieved accuracy at this level is nevertheless scarce, also owing to the fact that higher-level reference methods are often not available for standard periodic boundary condition supercell calculations. To this end, we present a study benchmarking semi-local and hybrid DFT against (renormalized) second-order perturbation theory (MP2,rPT2) as recently implemented in the FHI-aims package [1]. We make the efficient usage of the latter theories for oxide surfaces possible through a solid-state embedding framework, in which a central cluster region is described quantum mechanically, the long-range electrostatic interactions in the oxide are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the performance of the various levels of theories using the water-splitting reaction at ideal and defected TiO₂(110) surfaces as showcase. [1] X. Ren et al., *Phys. Rev. B* **88**, 035120 (2013)

MM 17.8 Mon 18:00 TRE Ma

Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors — ●GUO-XU ZHANG, ANTHONY M. REILLY, ALEXANDRE TKATCHENKO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound solids, ranging from wide-gap (10 eV) to narrow-gap (below 1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. The efficiency of our method and the accuracy of the calculated vdW parameters allows us to demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors. [1] Tkatchenko and Scheffler, *PRL* (2009); [2] Tkatchenko, DiStasio, Car, Scheffler, *PRL* (2012).

MM 17.9 Mon 18:15 TRE Ma

Adsorption at semiconductor surfaces - an energy analysis method — ●RALF TONNER and MARC RAUPACH — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg, Germany

The chemical bond is one of the most fundamental concepts in chemistry. Classifications such as covalent, ionic or metallic bonding are central in discussing trends in different compounds and predicting new reactivity. Several very helpful concepts and methods were developed to understand the chemical bond at surfaces.[1] The question about energetic contributions to surface chemical bonds on the other hand did not receive great attention although energy changes are the ultimate driving force in bond formation.

Starting from preliminary work by Philippsen and Baerends,[2] we implemented all terms of an Energy Decomposition Analysis (EDA) to obtain quantitative data about energetic contributions to chemical bonding in periodic systems. This periodic EDA method was applied to questions of chemisorption of organic molecules at semiconductor surfaces where it can shed light on the nature of the surface-adsorbate bonds.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, *Chemical Bonding at Surfaces and Interfaces*, Elsevier, Amsterdam, 2007; b) A. Groß, *Theoretical Surface Science*, Springer, Berlin, Heidelberg, 2009. [2] P. H. T. Philippsen, E. J. Baerends *J. Phys. Chem. B* 2006, 110, 12470.

MM 17.10 Mon 18:30 TRE Ma

Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions — ●JAN HERMANN, MATTHIAS SCHEFFLER, and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Different approaches to treating van der Waals (vdW) interactions in density-functional theory can be loosely divided into the atom-based and the ones based on non-local functionals. The first type comprises a range of methods from atom-pairwise additive schemes by Grimme to many-body dispersion (MBD) approach of Tkatchenko et al. Usually, these methods require precalculated atomic parameters and thus rely on information not explicitly contained in the electron density. The other category consists of nonlocal functionals either of the Langreth and Lundquist or the Vydrov and van Voorhis (VV) type. In these approaches, the vdW interaction is obtained as a functional of the electron density and at most a few tuning parameters are needed.

Here, we show that these two contrasting approaches can be synergistically combined. We use the polarizability from the nonlocal functional of VV within the MBD method of Tkatchenko et al. Such a combination is worthy for several reasons. First, it is an atom-centered approach with no atomic parameters. Second, it puts aside the problem of partitioning electron density between atoms, which can be problematic in some cases. Third, it enables more direct comparison of so far unrelated methods. Fourth, it highlights the idea of combining working elements from different approaches.

MM 18: Poster Session

Time: Monday 18:00–20:00

Location: P4

MM 18.1 Mon 18:00 P4
Microstructural Evolution of Nanoporous Gold During Coarsening — ●MARKUS ZIEHMER¹, KAIXIONG HU¹, KE WANG², JÜRGEN MARKMANN^{1,2}, and ERICA LILLEODDEN¹ — ¹Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Geesthacht, Germany — ²Hamburg University of Technology, Institute of Materials Physics and Technology, Hamburg, Germany

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

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

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

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

MM 18.2 Mon 18:00 P4
Thin-film cathodes for application in lithium ion batteries — ●MARTIN FIEDLER¹, FRANK BERKEMEIER¹, and GUIDO SCHMITZ² — ¹Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Institut für Materialwissenschaften, Universität Stuttgart, Heisenbergstr. 3, 70569 Stuttgart

Lithium Cobalt Oxide (LCO) and Lithium Iron Phosphate (LFP) powder material is commonly used in commercial lithium ion batteries. In this work, thin LCO and LFP films between 200 and 5500 nm in thickness are prepared by magnetron sputtering. After deposition, the layers are characterized by X-ray diffraction, transmission electron microscopy, and electrochemical techniques like cyclic voltammetry and chronopotentiometry. The influence of a negative substrate bias during sputter-deposition and of post annealing between 400 and 700°C is investigated, and it is found that the electrochemical performance of the layers significantly depends on both parameters. The preparation of films under optimized conditions gives smooth thin-film cathodes,

with a maximum thickness of 5500 nm and a lateral size of 45 cm². In case of LCO, this results in a lithium storage capacity up to 17 mAh. Despite their large thickness, the cathodes are mechanically stable and allow the investigation of transport kinetics without being influenced by interface effects. Moreover, they open the possibility to be used in technical lithium ion batteries, as substitutes for conventional powder cathodes.

MM 18.3 Mon 18:00 P4
Materials for all solid-state lithium-ion batteries — ●SUSANN NOWAK¹, FRANK BERKEMEIER² und GUIDO SCHMITZ¹ — ¹Institut für Materialwissenschaften, Heisenbergstr. 3, 70569 Stuttgart — ²Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

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

MM 18.4 Mon 18:00 P4
Sputter-deposited Thin-film Lithium Ion Batteries — ●FRANK BERKEMEIER, YASER HAMED, and FABIAN INKMANN — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

Electrochemical-active thin-film materials are deposited by sputter-deposition technique, with the aim to prepare an all-solid state thin-film lithium-ion battery. For this purpose silicon and tin are used as anode materials, while lithium cobalt oxide and lithium iron phosphate serve as cathodes. As an ion-conducting phase, thin-films of lithium phosphorous oxynitride (LiPON) are deposited. Via this setup, thin-film stacks with an overall thickness of less than 1µm are prepared, which are characterized by electrochemical techniques like impedance spectroscopy and cyclic voltammetry, as well as by transmission electron microscopy. It is shown that most of the thin-film cells show a reasonable charge-discharge behaviour, as well as a promising cycling

stability. Moreover it is demonstrated that by triggering a reaction between LiPON and a metallic layer like silver or magnesium, an interface reaction layer is formed that is capable of reversibly intercalate/deintercalate lithium. The structure and formation of this reaction layer is studied, and it is shown that in future thin-film cells this layer opens the possibility to substitute conventional thin-film cathodes – with the aim to increase the energy density and to decrease the internal resistance of the cells.

MM 18.5 Mon 18:00 P4

Nanostructured black silicon as anode for lithium-ion batteries — ●GIBA EK LEE^{1,2}, STEFAN L. SCHWEIZER², and RALF B. WEHRSPORN^{1,2} — ¹Fraunhofer Institute for Mechanics of Materials, Halle, Germany — ²Martin-Luther-University Halle-Wittenberg, Halle, Germany

It has been known for some time past that silicon can incorporate large amounts of Li with a specific capacity of 4200 mAh/g, about a factor of 11 larger than for state of the art graphite anodes. However, silicon and silicon-based negative electrodes exhibit huge volume expansion (ca. 320%) during lithiation/delithiation, resulting in mechanical disintegration of electrode and rapid capacity fading. Therefore, relaxation of the stress caused by the expansion and contraction of Li-Si alloy materials is important to obtain a good cycleability. Furthermore, the formation of solid electrolyte interphase (SEI) induced by decomposition of electrolyte hinders lithium ion movement during the Li-Si alloying/de-alloying, resulting in poor capacity retention upon cycles. In this study, we prepared well-ordered nanostructured black silicon arrays (nb-Si) on silicon substrate by gas chopping technique. The electrochemical properties of the nb-Si electrode were systematically investigated. The material characteristics have been analyzed by CV, SEM and TEM. The performance of nb-Si electrode has been examined by galvanostatic charge/discharge cycling. In order to understand the correlation between surface condition and Li-Si alloying, we have investigated the surface composition of nb-Si electrode before and after pretreatment by means of high resolution XPS as well

MM 18.6 Mon 18:00 P4

In-situ TEM studies of nanostructured Mg based hydrides at elevated hydrogen pressures of 1 bar — ●ALEXANDER SURREY^{1,2}, LUDWIG SCHULTZ^{1,2}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — ²TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

In the search of materials that are potentially applicable as solid-state hydrogen storage materials in the mobile and stationary sector, MgH₂ is considered one of the most promising hydrides due to both its relatively high gravimetric storage density of 7.7 wt.-% and its high abundance. However, the thermodynamic and kinetic properties of intrinsic MgH₂ impede a practical application. Here, nanostructured hydrides have been shown to reveal improved (de)hydrogenation properties. During structural characterization utilizing conventional TEM, however, MgH₂ degrades fast upon the irradiation with the imaging electron beam due to radiolysis in vacuum and as a consequence, the hydride phase cannot be studied at highest resolution. To overcome this problem we explore the possibility to investigate Mg based hydrides by in-situ TEM at elevated H₂ pressures (1 bar) and temperatures (up to 300°C) using a so called nanoreactor that was recently developed by Henny Zandbergen at the TU Delft. This allows to study the dehydrogenation as well as the hydrogenation reaction at the nanoscale under working conditions. We present multi-slice HRTEM contrast simulations to show the possibilities and limitations of this new nanoreactor. Such simulations may be valuable to pre-evaluate future experiments.

MM 18.7 Mon 18:00 P4

Influence of temperature on hydrogen induced surface modification on Gd(0001) islands — ●SAMUEL KÖNIGSHOFEN, SARA WANJELIK, and MATHIAS GETZLAFF — Institute of Applied Physics, University of Düsseldorf

The adsorption of hydrogen on metal surfaces is of great interest in fundamental research and also applied science due to its importance for technology and material science. Although there has been research for many years, the subsequent hydride formation and especially their initial behavior is not completely understood yet. Here we present measurements, carried out by scanning tunneling microscopy, on gadolinium islands of 100-400 nm size and a few nanometers in height. The islands are grown on a W(110) surface. The initial stage of hydride for-

mation and the localization of its occurrence will be of special interest. Further, the appearance and change of the hydrides due to heating of the sample has been observed. The steps of the temperature variation are in the range of a few hundred kelvin starting at room temperature. Additionally, the time dependence of the formation will be discussed. The known occurrence of disc-like island and formation of ramps on Gd thin films due to hydrogen adsorption will be compared to the investigated hydride characteristics of Gd islands.

MM 18.8 Mon 18:00 P4

Preparation of a Ta(110) surface for hydrogen absorption — ●SEBASTIAN SCHLEICHER, SARA WANJELIK, and MATHIAS GETZLAFF — Institut für Angewandte Physik, Universität Düsseldorf, Deutschland

Hydrogen in metals has attracted a lot of attention in the past decades. On the one hand this is caused by the technical application as hydrogen storage. On the other hand metal hydrogen systems are of great interest from a fundamental point of view. In our study we investigate hydrogen on adsorption and absorption in a Ta(110) crystal which requires careful cleaning as preparation for any measurement on the Tantalum surface. The cleaning procedures include heating up to 2900°C, annealing in an oxygen atmosphere and sputtering with a sputter ion source to remove impurities. The subsequently observed superstructure remains unaffected and may show a reconstructed pattern of a clean Tantalum surface. Measurements are performed by means of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) under ultrahigh vacuum conditions.

MM 18.9 Mon 18:00 P4

A new additive-assisted synthesis route and electrochemical properties of olivine LiCoPO₄ — ●CHRISTOPH NEEF¹, HANS-PETER MEYER², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg — ²Institut für Geowissenschaften, Universität Heidelberg, D-69120 Heidelberg

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

MM 18.10 Mon 18:00 P4

Pathway to mechanically stable magnetocaloric cycling materials — ●ALEXANDER FUNK^{1,3}, ANJA WASKE¹, MARIA KRAUTZ², BRUNO WEISE^{1,3}, KONSTANTIN SKOKOV⁴, and JÜRGEN ECKERT¹ — ¹Institute for Complex Materials, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — ²Institute for Metallic Materials, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — ³Institute for Material Science, TU Dresden, Helmholtzstraße 7, 01069 Dresden, Germany — ⁴Material Science, TU Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

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

References:

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

MM 18.11 Mon 18:00 P4

Graphitization and interface bonding in carbon-bonded alumina ceramics — ●TORSTEN WEISSBACH, MASUD ALAM, CHRISTIAN

RÖDER, LILIT AMIRKHANYAN, and JENS KORTUS — Institut f. Theoretische Physik, TU Bergakademie Freiberg, 09596 Freiberg

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

[1] Markus Emmel et al., *Ceramics International* (2012)

[2] Christian Röder et al., *Journal of Raman Spectroscopy*, accepted

[3] Stefan Grimme, *Journal of Computational Chemistry* (2006)

MM 18.12 Mon 18:00 P4

Light-driven rotation of chiral, screw-like microstructures in a fluidic environment — ●LINDSEY JE ANDERSON¹, SILKE KIRCHNER¹, DEBORA SCHAMEL², PEER FISCHER², THEOBALD LOMÜLLER¹, and JOCHEN FELDMANN¹ — ¹Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universität München, Amalienstr. 54 80799 Munich, Germany — ²Max Planck Institute for Intelligent Systems, Heisenbergstr. 3 70569 Stuttgart, Germany

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

MM 18.13 Mon 18:00 P4

Phase-field simulation of interdiffusion-limited coarsening in Ni-base superalloys under applied loads — ●LESLIE MUSHONGERA, MICHEAL FLECK, JULIA KUNDIN, and HEIKE EMMERICH — University of Bayreuth

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

MM 18.14 Mon 18:00 P4

Continuum modelling of grain boundary wetting — ●VENKATA SAI PAVAN KUMAR BHOGIREDDY¹, FABIAN TWISTE¹, CHI-DZU NGUYEN¹, CLAAS HÜTER¹, ROBERT SPATSCHEK¹, JÖRG NEUGEBAUER¹, ALAIN KARMA², and EFIM BRENER³ — ¹Max Planck Institut für Eisenforschung, D-40237, Düsseldorf, Germany — ²Physics Department, Northeastern University, Boston, 02115, USA — ³Peter Grünberg Institut, Forschungszentrum Jülich, D-52425, Jülich, Germany

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

phase field model based on the multi-obstacle potential to capture the premelting transition.

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

MM 18.15 Mon 18:00 P4

Molecular Dynamic Simulation of atomic deposition between MnAs cluster — ●ANDREAS RÜHL and CHRISTIAN HEILIGER — I. Physikalisches Institut, Justus Liebig Universität Giessen, D-35392 Giessen, Germany

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

MM 18.16 Mon 18:00 P4

Modeling phase transformations in binary alloys for eutectic systems — ●MUHAMMAD AJMAL CHOUDHARY¹, JULIA KUNDIN¹, MARTIN OETTEL², and HEIKE EMMERICH¹ — ¹Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth. — ²Institut für Angewandte Physik, Universität Tübingen, D-72076 Tübingen.

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

MM 18.17 Mon 18:00 P4

Effect of surfaces and interfaces on elastic properties of transition metals studied by DFT and EAM — ●TOBIAS KLÖFFEL¹, ERIK BITZEK², and BERND MEYER¹ — ¹Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — ²Department of Materials Science and Engineering, WW 1: General Materials Properties, FAU Erlangen-Nürnberg

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

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

MM 18.18 Mon 18:00 P4

Simulation of the elastic properties of nanomechanical beam and membrane resonators — ●KRISTIAN SCHOLZ, THOMAS

MÖLLER, DANIEL MUTTER, MARKUS RING, RALF SCHMID, MARTIN VÖGELE, and PETER NIELABA — Physics Department, University of Konstanz, Germany

The oscillation behaviour of nanomechanical resonators in the form of doubly clamped beams and clamped membranes is investigated by molecular dynamics simulations. After setting up the initial structure, the end points of the beams or the outer border of the membranes, respectively, are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the structures. Besides varying the size of the structures, the effects of temperature, external stretching fields, cavities and crystal faults are explored. The results show a decrease of the oscillation frequencies and an increase of the damping coefficient with rising temperature, a strong increase of the frequencies with external stress (stretching), a decrease of frequencies with size and an increase of the damping coefficient when adding cavities to the structures. It is also possible to observe the dissipation of energy from the collective oscillation of the structures into thermal energy of the degrees of freedom of the constituting atoms. Different materials (e.g. *Si*, *Si₃N₄* and *NiTi* memory alloys) are explored as well. In order to explore quantum effects in the low temperature regime path integral Monte Carlo simulations are performed.

MM 18.19 Mon 18:00 P4

Heat capacity of Al₃FeSi₂: Quasiharmonic approximation versus Neumann-Kopp rule and measurement — ●LILIT AMIRKHANYAN¹, TORSTEN WEISSBACH¹, THOMAS GRUBER¹, OLGA FABRICHNAYA², TILO ZIENERT², and JENS KORTUS¹ — ¹Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09596 Freiberg, Germany — ²Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Straße 5, D-09595 Freiberg, Germany

Thermodynamic databases are an important tool for the simulation of solid state reactions and phase diagrams. In cases when the thermodynamic data are not available for a certain compound, they are calculated in approximation from elemental data (Neumann-Kopp rule [1]). Here we compare experimental DSC data with the Neumann-Kopp rule and first-principles calculations based on DFT and the quasiharmonic approximation. The compound in question is the τ_4 -AlFeSi phase, a ternary light-metal alloy from the Aluminium-rich side of the system. We show that the DFT-QHA calculations are in good accord with the measured heat capacity (c_p), while the N-K rule suffers several shortcomings.

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

MM 18.20 Mon 18:00 P4

Temperature dependence of the elastic constants of W: An ab-initio study — ●THOMAS DENG^{1,2}, JÜRGEN SPITALER¹, LORENZ ROMANER¹, and PETER PUSCHNIG² — ¹Materials Center Leoben Forschung GmbH — ²Karl-Franzens-Universität Graz, Institut für Physik

Two different ab-initio approaches for calculating the temperature dependence of the elastic constants of W are investigated. On the one hand the influence of temperature is taken into account only through the volume expansion. Here, thermal expansion can either be taken from experiment or determined theoretically within the quasiharmonic approximation. On the other hand the temperature dependence can explicitly be determined by calculating the free energy as a function of strain. To this end, the phonon density of states is calculated for a set of strained structures. The results from both approaches are compared with each other and it is assessed how they perform in terms of computational effort and accuracy and last but not least how well they agree with experimental values.

MM 18.21 Mon 18:00 P4

The F Center in Lithium Fluoride revisited: comparison of solid-state physics and quantum-chemistry approaches — ●FERENC KARSAI¹, PAUL TIWALD¹, JOACHIM BURGDÖRFER¹, PETER BLAHA¹, LUDGER WIRTZ², ROBERT LASKOWSKI¹, FABIEN TRAN¹, DAVID KOLLER¹, and STEFANIE GRÄFE¹ — ¹Vienna University of Technology, Vienna, Austria — ²University of Luxembourg, Luxembourg, Luxembourg

The F-type color-center in LiF is an old prototype problem where an electron is trapped at a vacant anion site. In an intuitive picture the defect electron can be approximately described as a particle in the box. We present a comparison of the physicist's approach (peri-

odic supercell-approach with various DFT-functionals, GW and Bethe-Salpeter methods) and the quantum-chemist's approach (embedded-cluster approach with wave-function methods such as CASPT2). In both cases, we observe strong excitonic effects due to the strong localization of the defect in agreement with the simple particle in box picture. We also find that the calculated absorption spectra from both approaches are in unprecedented agreement with experiment.

MM 18.22 Mon 18:00 P4

On low-energy electronic excitations in the Ti_{1-x}Al_xN-system — ●SIMON LAMOWSKI, TORSTEN WEISSBACH, and JENS KORTUS — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, 09599 Freiberg, Germany

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

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

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

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

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

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

MM 18.23 Mon 18:00 P4

Atomistic modelling of phase transitions in Ti-Ta high-temperature shape memory alloys — ●TANMOY CHAKRABORTY, JUTTA ROGAL, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

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

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

MM 18.24 Mon 18:00 P4

Range Separated Functionals in the Density Functional Based Tight Binding Method — ●VITALIJ LUTSKER and THOMAS A. NIEHAUS — Universität Regensburg

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

MM 18.25 Mon 18:00 P4

Large scale Born-Oppenheimer MD with full local orbital optimization — ●SIMON DUBOIS^{1,2} and MIKE PAYNE² — ¹Institute of Condensed Matter and Nanosciences, UCL, Louvain-La-Neuve, Belgium — ²Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

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

MM 18.26 Mon 18:00 P4

C, N and H binding energies in Fe₂Nb Laves — ●ALVIN NOE LADINES, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — ICAMS, Ruhr Universität Bochum, Germany

The family of Laves phases are interesting from a technological point of view because of their capability for hydrogen storage and their strengthening effect in steel. Although their bulk properties are well understood, the solubility of light elements in these compounds is still unclear. This is due in part to their complex defect structure and the limitations of current experimental techniques for light elements. In this study, we use density functional theory (DFT) to calculate the solubility of C, N and H at the different interstitial sites in the Fe₂Nb C14 Laves phase. Our results suggest that the light elements prefer the voids centered at the triangles shared by two adjacent tetrahedral elements over the centers of these tetrahedra due to the slightly larger volume. Moreover, the binding energies are also dependent on the number of Nb nearest neighbors which is consistent with the high affinity of C, N and H to Nb. Our results suggest a considerable solubility of N and H in Fe₂Nb. For C, we observe a weaker solubility which we attribute to the increased strain that is apparent as increased bond lengths.

MM 18.27 Mon 18:00 P4

Electromagnetic field distribution in composite materials: Are there hot spots? — ●CINTIA HARTMANN¹, BÉATRICE HALLOUET¹, ROMANUS DYCZIJ-EDLINGER², and ROLF PELSTER¹ — ¹Fachrichtung 7.2 Experimentalphysik Universität des Saarlandes Campus E2 6 D-66123 Saarbrücken — ²Lehrstuhl für Theoretische Elektrotechnik Universität des Saarlandes Campus C6 3 D-66123 Saarbrücken

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

MM 18.28 Mon 18:00 P4

Bestimmung der Nachweisgrenze bei der Tiefenprofilierung von Fluor in TiAl mittels PIGE — ●DANIEL BRENNER¹, HANS-EBERHARD ZSCHAU², SVEN NEVE¹ und LOTHAR SCHMIDT¹ — ¹Institut für Kernphysik, Frankfurt a.M., Deutschland — ²Dechema-Forschungsinstitut, Frankfurt a.M., Deutschland

Die Modifizierung der Oberflächen von Titan-Aluminium-Legierungen mit Fluor verbessert die Oxidationsbeständigkeit bei hohen Temperaturen. Bei einem neuen Verfahren des Recyclings des Werkstoffs werden geringe Mengen CaF₂ zugesetzt. Auch dies könnte zu einem erfolgreichen Oxidationsschutz führen.

Um einen erfolgreichen Halogeneffekt für geringe Konzentrationen von Fluor nachweisen oder widerlegen zu können, muss Fluor bei Konzentrationen im ppm-Bereich zerstörungsfrei nachgewiesen werden können. Dazu wurden TiAl-Proben mit geringen Mengen Fluor oberflächennah implantiert. Durch Mehrfachimplantationen kann ein Bereich annähernd konstanter Fluor-Konzentration realisiert werden. Die Technik der Proton Induced Gamma Emission (PIGE) diente zum Nachweis der implantierten Profile. Die Nachweisgrenze unter den Bedingungen der zerstörungsfreien Tiefenprofilierung des bisher üblichen

Messsystems mit NaI-Detektor und VKA wurde auf 400 ppm bestimmt und nach Umstieg auf digitale Datenaufnahme weiter verbessert. Es wurden sowohl mit Fluor implantierte TiAl-Proben, als auch Proben aus recyceltem TiAl untersucht.

MM 18.29 Mon 18:00 P4

Instabilities during frictional sliding — ●MARC WEIKAMP¹, ROBERT SPATSCHKE¹, EFIM BRENER^{2,3}, ERAN BOUCHBINDER³, and YOHAÏ BAR SINAI³ — ¹Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — ²Peter Grünberg Institut, Forschungszentrum Jülich, D-52425 Jülich, Germany — ³Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100, Israel

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

MM 18.30 Mon 18:00 P4

In-situ TEM fracture tests of nanoscale multilayers — ●CHRISTIAN MECKENHÄUSER, ANDREAS KELLING, INGA KNORR, TOBIAS LIESE, HANS-ULRICH KREBS, and CYNTHIA A. VOLKERT — Institute for Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany

Nanocomposite materials are commonly used in many different applications due to their unique combinations of material properties. Here, we try to understand the mechanism of fracture in nanocomposites and the influences of interfaces on fracture in order to learn how to separate nanoscale materials efficiently. By varying the layer thicknesses a possible length scale depend behavior of fracture in nanoscale multilayer systems can be tested. The multilayers consist of nanocrystalline Ti and amorphous ZrO₂, both deposited by pulsed laser deposition. The mechanical properties of the multilayer samples have been determined using Berkovich indentation and microcompression tests. The interfaces of the multilayer system are very sharp and smooth and the layer thicknesses of each material can be varied between 10 and 100 nm resulting in a perfect set of different samples for the fracture tests. We deform these multilayers with a specially designed in-situ setup inside a TEM using an STM holder which allows for stable and controllable crack growth. Initial studies on samples with 100 nm thick layers show that the cracks form at a notch created with the FIB and run through the middle of a Ti layer. The crack may jump to a neighboring Ti layer by forming a shear band in the intervening ZrO₂ layer. In this presentation we will show preliminary results of fracture tests.

MM 18.31 Mon 18:00 P4

Structure and thermal stability of HPT-processed Cu-16 at.%Al — ●NAZAR IBRAHIM, MARTIN PETERLECHNER, SERGIY DIVINSKI, and GERHARD WILDE — Institute of Materials Physics, Westfälische Wilhelms-University Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Severe plastic deformation is an effective tool for production ultra-fine grained materials with extraordinary mechanical properties, corresponding to a high strength and relatively good ductility. In this work, structure modification by high pressure torsion (HPT) and the thermal stability of the resulting microstructure are investigated for the Cu16 at.% Al alloy. For this alloy, a propensity for five-fold twinning has recently been reported [X.H. An, et al., Scripta Materialia 64 (2011) 249]. Disks with a thickness of 0.8 mm and diameter of 10 mm were processed via HPT for 2, 5, 10 and 20 revolutions at room temperature under hydrostatic pressure levels of 2, 4 and 6 GPa and a rotational speed of 1 rpm. Structural and thermal analyses were carried out using X-ray diffraction, transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). The DSC experi-

ments using constant heating rates showed two exothermic peaks in the temperature range from 30°C to 450°C. After HPT a highly distorted structure was observed, including dislocations, fragmented grains and twins. Due to the low stacking fault energy in Cu₈Al₁₆, twinning makes a significant contribution to plasticity during HPT. The results are discussed with respect to the reported five-fold twinning in this alloy.

MM 18.32 Mon 18:00 P4

Microstructural analysis of the creep behavior of directionally solidified eutectic NiAl-Cr — ●ANTJE KRÜGER, MICHAEL KLIMENKOV, and ANTON MÖSLANG — Institute for Applied Materials - Applied Materials Physics, Karlsruhe Institute of Technology (KIT)

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

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

The authors thank the Helmholtz association for financial support.

MM 18.33 Mon 18:00 P4

PAC studies of uniaxial compressive stressed zinc, titanium, rutile, Ti₂AlN, and Nb₂AlC — ●CHRISTOPH BRÜSEWITZ¹, DANIEL JÜRGENS¹, ULRICH VETTER¹, HANS HOFSSÄSS¹, and MICHEL W. BARSOM² — ¹II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — ²Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

Polycrystalline zinc, titanium, rutile, and the MAX phases Ti₂AlN and Nb₂AlC were studied with the perturbed angular correlation (PAC) method using ¹¹¹In/¹¹¹Cd as probe atom. The electric field gradient (EFG) at room temperature was studied as function of mechanical deformation caused by a uniaxial compressive load. A reversible and an irreversible increase in the distribution width of the EFG, visible as a damping of the PAC spectrum, were found under load and after releasing the load, respectively. Annihilation of dislocations, in agreement with the proposed incipient kink band (IKB) mechanism, as well as elastic deformation are considered to contribute to the reversible behavior. The irreversible behavior is caused by a permanent increase in dislocation and point defect density. The deformation induced broadening of the EFG can be recovered by post-annealing of the deformed sample.

MM 18.34 Mon 18:00 P4

In-situ TEM deformation of Ti₃SiC₂- MAX phase — ●MONA-CHRISTIN MAASS, BURKHARD ROOS, and CYNTHIA A. VOLKERT — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany

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

In-situ TEM experiments are performed to examine the plastic deformation of Ti₃SiC₂, where dislocation motion is strongly constrained in the basal planes, and to gain insights into the 2-dimensional dynamics of dislocations. For these experiments samples were prepared by conventional thinning with dimpling and Ar ion milling, and also by FIB milling. The samples contained an initial high density of dislocations and were deformed in-situ by loading them with a piezo actuated tungsten tip. These in-situ experiments showed that dislocations move under loading and are able to leave the sample at its free surfaces. Based

on crystallographic investigations and TEM post-mortem analysis the slip planes and slip directions of the dislocations and their interactions with existing defects in Ti₃SiC₂ is discussed. Although these observations are specific to Ti₃SiC₂, other MAX phases are likely to behave similarly because they all have similar layered, hexagonal structures.

MM 18.35 Mon 18:00 P4

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

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

MM 18.36 Mon 18:00 P4

Waiting time statistics indicating crossover from 3D uncorrelated nano shear bands to cooperative shear motion — JON-OLAF KRISPONEIT, ●SEBASTIAN PITIKARIS, KARINA E. AVILA, STEFAN KÜCHEMANN, ANTJE KRÜGER und KONRAD SAMWER — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We investigated the post-elastic creep deformation of Pd_{77.5}Cu₆Si_{16.5} metallic glass ribbons via Dynamical Mechanical Analysis, i.e. we recorded its strain response over time after exerting a uniaxial stress jump. Macroscopically, one observes a smooth strain curve comprising of elastic, anelastic and plastic contributions. On a finer scale, however, the creep curve is made up of steplike jumps rather than proceeding continuously. We approach the statistical properties of the underlying slip events using a novel waiting time analysis. These show a power law distribution similar to those observed for other systems exhibiting avalanche dynamics e.g. Barkhausen noise or fracture in crystals. In long-time experiments we observed a crossover between two distinct power law regimes. We ascribe the first regime to the stress-assisted formation of 3D independent avalanches of shear transformation zones, the fundamental microscopic unit of deformation. The transition to a second power-law regime indicates the onset of cooperative 2D nano shear band motion. We acknowledge financial support for this work by DFG via SFB 602 and FOR 1394 and the German-Israeli Foundation.

MM 18.37 Mon 18:00 P4

Electronic properties of metallic gallium up to 4 GPa as studied with new anvil-cell NMR — ●THOMAS MEIER and JÜRGEN HAASE — Universität Leipzig, Institut für Experimentelle Physik II

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

MM 18.38 Mon 18:00 P4

Hardness measurements of shear bands in the bulk metallic glass Pd₄₀Ni₄₀P₂₀ by Nanoindentation — ●NIKLAS NOLLMANN,

JÖRN LEUTHOLD, and GERHARD WILDE — WWU Münster, Deutschland

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

MM 18.39 Mon 18:00 P4

Effect of shear localization on atomic transport and mechanical damping in a Pd40Ni40P20 bulk metallic glass — ●ISABELLE

BINKOWSKI¹, IGOR S. GOLOVIN², SERGIY V. DIVINSKI¹, and GERHARD WILDE¹ — ¹1- Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — ²2- Technological University 'MISIS', Leninsky ave.4, 119049 Moscow, Russia

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

Financial support of DFG and RFBR (project 13-03-91330/13) are acknowledged.

MM 19: Invited Talk (Hauptvortrag) Maier

Time: Tuesday 9:30–10:00

Location: BAR 205

Invited Talk

MM 19.1 Tue 9:30 BAR 205

Size effects on ion transport and energy storage in nanomaterials — ●JOACHIM MAIER — Max Planck Institute for Solid State Research, Stuttgart, Germany

Mobile ions enable a palette of applications in particular in the field of energy research and cannot be rendered dispensable by using electrons. Typical examples are fuel cells and batteries. Here nanoionics can have a substantial impact.

Not only can the introduction of interfaces and the variation of their spacing drastically vary conductivities, also qualitative changes can be achieved: insulators can be turned into conductors, electronic conduc-

tors into ion conductors, anion into cation conductors and interstitial into vacancy conductors. The use of true size effects leads to the generation of artificial mesoscopic ion conductors.

Size effects can be of direct relevance for electrochemical devices such as lithium-based batteries. Here effects on cell voltage and ion transport in the electrolytes are considered. Size effects lead, in addition to conductivity anomalies, also to storage anomaly. It is shown that in composites lithium can be accommodated by a "job-sharing" mechanism even though none of the constituted phase may be able to do so. Besides pronouncing the materials science implications, the underlying thermodynamic concepts are emphasized.

MM 20: Topical Session: Nanomechanics of nanostructured materials and systems IV - Tribology/Composites

Time: Tuesday 10:15–12:00

Location: IFW A

Topical Talk

MM 20.1 Tue 10:15 IFW A

Nanometer-scale plasticity of (amorphous) metallic surfaces — ●ARNAUD CARON, JOHANNES MAURER, and ROLAND BENNEWITZ — INM Leibniz-Institute for New Materials, Campus D2.2, 66123 Saarbrücken, Germany

The sub-micrometer-scale plastic deformation of Pt(111) and Pt57.5Cu14.7Ni5.3P22.5 metallic glass is discrete in nature and can be rationalized by the respective mechanisms for plastic deformation: burst-like activation and sliding of dislocation for crystalline metals and localized shear banding for metallic glasses. The discrete character of plastic deformation is conserved at the nm-scale for Pt(111). In contrast we observe a homogeneous flow in the case of Pt57.5Cu14.7Ni5.3P22.5 metallic glass at the nm-scale. On the one hand, the nm-scale plastic deformation of Pt(111) is mediated by the homogeneous nucleation and gliding of single dislocations. On the other hand, the nm-scale plastic deformation of Pt57.5Cu14.7Ni5.3P22.5 metallic glass involves the collaborative flow of structural unit, such as in the flow of viscous liquids and can be referred to as a structural collapse. Likewise, the nm-scale wear behaviour of Pt(111) occurs by dislocation-mediated homogeneous plastic deformation. In contrast, the wear of Pt57.5Cu14.7Ni5.3P22.5 metallic glass occurs through localized plastic deformation in shear bands that merge together in a single shear zone above a critical load and corresponds to the shear softening of metallic glasses.

MM 20.2 Tue 10:45 IFW A

Grain size and orientation evolution of high-purity copper un-

der reciprocating tribological loading — ●CHRISTIAN GREINER and ZHILONG LIU — IAM-ZBS, Karlsruhe Institute of Technology, Karlsruhe, Germany

One of the key questions in tribology is to correlate a material's microstructure with its friction and wear properties. However, there is still a significant lack of knowledge about the mechanisms for the evolution of the microstructure under a tribological load.

A reciprocating motion and high-purity copper in contact with a sapphire sphere was investigated. With an annealed initial microstructure, the energy dissipated during the sliding motion was varied by increasing the sliding distance up to several meters. A dual-beam microscopy system (FIB and SEM) was used to investigate the resulting grain size and to perform EBSD and (S)TEM measurements to follow the evolution of the microstructure in the wear track thoroughly. Results for the microstructure evolution, e.g. grain size and preferred orientation, with the sliding distance will be presented.

A long term goal of this study is to develop a model description for the microstructural changes in view of energy and mechanics in order to understand these changes and their influence on the tribological properties. In the future, this might allow for tailored microstructures combining low friction forces and very small wear rates.

MM 20.3 Tue 11:00 IFW A

Nanoporous gold - polymer composites with strength and conductivity — ●KE WANG¹ and JÖRG WEISSMÜLLER^{1,2} — ¹Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany — ²Institut für Werk-

stoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Nanoporous metal synthesis via dealloying provides mm- or cm-sized monolithic samples consisting of a homogeneous network structure of nanoscale "ligaments" with uniform size that can be controlled down to below 10 nm. The strength of the ligaments increases with decreasing size, attaining the theoretical strength at ligament diameters in the lower nanometer region. Here, we explore a novel materials design strategy that combines this high-strength and uniform metallic network structure with an interpenetrating polymer phase to obtain a strong, lightweight composite material. The porous metal was vacuum-impregnated with epoxy resin and tested for microhardness, macroscopic tensile and compressive stress-strain behavior. The results demonstrate that impregnation with a polymer is an efficient way of reducing the density change during plastic flow under uniaxial load. The composite is ductile in tension and compression, its strength considerably exceeds that of each of the constituent phases, and its electric conductivity reaches 1% of that of high-purity massive copper. The finding validates a novel materials design strategy that exploits the trend of "smaller is stronger" in metal nanostructures by incorporating them as reinforcement into a bulk composite material.

MM 20.4 Tue 11:15 IFW A

Micromechanical characterization of nanoporous gold/epoxy composites — ●KAIXIONG HU¹, KE WANG², DANIEL KUPKA¹, MARKUS ZIEHMER¹, and ERICA LILLEODDEN¹ — ¹Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht — ²Institute of Materials Physics and Technology, Hamburg University of Technology

Nanoporous gold displays tunable mechanical behavior through the variation of internal length-scales, but it is severely limited by its lack of ductility in tension. By infiltrating the porous structure with epoxy, a composite material with tensile ductility and enhanced flow stress is achieved. Importantly, the infiltration of epoxy offers an advantage for 3D tomographic analysis by allowing "clean" cross sectioning with a focused ion beam. The resultant 3D reconstructions can be used to quantify characteristic structural parameters, and as direct input

for finite element simulations of deformation. This, in turn, allows an improved description of the structure-property relations controlling this unique material. In the presented work, we have carried out a study of the micromechanical investigation of the nanoporous gold-epoxy composite using nanoindentation-based testing methods and finite element simulations, along with 3D tomographic characterization of the undeformed and deformed material. Results reveal how the 3D microstructure of the composite influences its mechanical behavior, and are discussed in terms of size-dependent plasticity and classical scaling laws for porous materials.

Topical Talk

MM 20.5 Tue 11:30 IFW A

Linking experiments and simulations to understand third body formation of tribologically stressed surfaces — ●MARTIN DIENWIEBEL^{1,2}, PANTCHO STOYANOV^{1,2}, PEDRO A. ROMERO^{1,2}, ROLF MERZ³, PRISKA STEMMER⁴, and MICHAEL MOSELER^{2,5} — ¹Karlsruhe Institute of Technology, MicroTribology Center, IAM-ZBS, Karlsruhe, Germany — ²Fraunhofer IWM, Freiburg, Germany — ³IFOS GmbH, Kaiserslautern, Germany — ⁴University Duisburg-Essen, Duisburg, Germany — ⁵University of Freiburg, Freiburg, Germany

In the present work we aim to link tribometry with atomistic simulations in order to improve our understanding of nanoscale interfacial processes of a tungsten-carbon-hydrogen tribo couple. Sliding induces severe changes of the material with respect to topography, composition and microstructure ("third body", [1]). Experiments were performed using a novel experimental platform for the on-line correlation of friction, wear and topography under lubricated sliding [1]. Then, in order to elucidate the atomistic level processes which contribute to the observed microstructural evolution in the experiments, classical molecular dynamics are performed employing a bond order potential for the Tungsten-Carbon-Hydrogen system. The combined experimental and simulation data allowed a look at the third body formation of metals (tungsten), ceramics (WC) [3,4] and diamond-like carbon coatings [5].

[1] M. Godet, *Wear*, 100 (1984) 437-452. [2] S. Korres, M. Dienwiebel, *Rev. Sci. Instrum.*, **81** (2010) 063904. [3] P. Stoyanov et al., *Tribol. Lett.*, **50** (2013) 67-80. [4] P. Stoyanov et al., *ACS Appl. Mat. Int.*, **5** (2013) 6123-6135. [5] P. Stoyanov et al., *Acta mater.*, accepted (2013)

MM 21: Topical Session: Thermodynamics at the nano scale I - Kinetics, nucleation, grain growth, segregation

Time: Tuesday 10:15–11:30

Location: BAR 205

Topical Talk

MM 21.1 Tue 10:15 BAR 205

Nucleation and growth in small systems — ●CHRISTOPH DELLAGO — University of Vienna, Vienna, Austria

Under suitable conditions, first order phase transitions such as the freezing of a liquid or the structural transformation of a solid occur via a nucleation and growth mechanism, in which a nucleus of the stable phase is formed in the metastable phase. For systems with sizes in the nanometer regime, the nucleation mechanism and its kinetics are strongly affected by finite size effects. I will address this issue using melting/freezing of gold nanoparticles and the Wurtzite-to-rocksalt transition in CdSe nanocrystals as illustrative examples. Based on the results of transition path sampling simulations, I provide a picture of the transition mechanism paying particular attention to the structure of the critical nuclei. The role of the reaction coordinate in the investigation of the transition mechanism is discussed.

MM 21.2 Tue 10:45 BAR 205

Observing steady-state coarsening: From nanocrystalline to normal grain growth — ●DANA ZÖLLNER and PETER STREITENBERGER — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

It is well-known that normal grain growth is characterized by a parabolic growth law and self-similar scaling resulting in a universal, time-independent grain size distribution as well as in a self-similar topology of the polycrystalline grain microstructure. In the present work we show by theoretical considerations and modified Potts model simulations that self-similarity is also a feature of junction controlled grain growth as it can be found in nanocrystalline materials.

To this aim, the influence of the grain junctions - boundary faces,

triple lines and quadruple points - on the growth kinetics is analyzed by attributing each type of boundary junction an own specific energy and mobility. This strategy results in nine size-dependent types of growth kinetics, each characterized by a self-similar scaling form of the growth law and corresponding self-similar grain size distributions. For the three limiting cases of grain growth controlled by the specific grain boundary energy in conjunction with the mobility of grain boundaries, triple lines or quadruple points the analytical results are in good agreement with those obtained by Potts model simulations. In particular, we show that triple and quadruple junction controlled coarsening is characterized by a series of quasi-steady-states reaching for long-time annealing the characteristics of normal grain growth.

MM 21.3 Tue 11:00 BAR 205

Segregation at and structure of iron grain boundaries using parameterized electronic description. — ●GEORG K. H. MADSEN¹, JINGLIANG WANG¹, NICHOLAS HATCHER^{1,2}, and RALF DRAUTZ¹ — ¹ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²QuesTek Innovations LLC, Evanston, IL 60201, USA

We employ a recently developed iron carbon orthogonal tight-binding model of grain boundaries (GBs) in the iron-carbon system. Bulk electron states are captured in this model as it is applied to systems containing over 5,000 ferromagnetic atoms. A strategy for a systematic screening of grain boundary energies has been applied to BCC-Fe. We show how the Fe-Fe tight binding model is able to pre-screen the rigorous coincidence site lattice GBs and apply it to calculate the stable $\Sigma < 15$ GBs in α -Fe.

The properties of carbon near and on the $\Sigma 5$ (310)[001] symmetric tilt GB are calculated and it is found that a carbon atom lowers the GB energy by 0.29 eV/atom in accordance with the DFT value

of 0.23 eV. Carbon segregation to the GB is analyzed, and we find an energy barrier of 0.92 eV for carbon to segregate to the carbon-free interface while segregation to a fully-filled interface is disfavored. We isolate two different mechanisms governing carbon's behavior in iron: a volumetric strain which increases the energy of carbon in interstitial α -iron and a non-strained local bonding which stabilizes carbon at the GB.

MM 21.4 Tue 11:15 BAR 205

Solid state amorphization of thin metal films embedded in bulk metallic glass — ●TOBIAS BRINK¹, DANIEL ŞOPU^{1,2}, and KARSTEN ALBE¹ — ¹Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — ²now at ICAMS, Ruhr-Universität Bochum, Germany

Metals commonly appear in crystalline phases. Even thin films of metal stay crystalline on a variety of substrates. In contrast, it was

recently observed experimentally, that thin metal layers embedded in a bulk metallic glass matrix become amorphous if they are thin enough (Ghafari *et al.*, Appl. Phys. Lett. **100** (2012), 203108). The resulting multilayer systems have possible applications in the realm of materials for magnetic tunnel junctions, among others. We reproduced this effect in a series of molecular dynamics simulations and investigated the driving force behind it. We show that thin amorphous metal nanolayers in our model system are thermodynamically stable. We present a model based on a competition between the excess energy of the amorphous phase and the interface energy. We show that the glass–glass interface has lower potential energy than the corresponding crystal–glass interface. Our model correctly predicts the critical thickness under which amorphization occurs. These results suggest that other technologically relevant systems with amorphization of metallic nanolayers may exist. The results are also of interest for the study of crystalline phases in bulk metallic glasses.

MM 22: Mechanical properties I - Plastic deformation & fracture

Time: Tuesday 10:15–11:45

Location: IFW B

MM 22.1 Tue 10:15 IFW B

Ductile-to-brittle transition in metallic glasses under cryogenic cooling — ●MINQIANG JIANG — State Key Laboratory of Non-linear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, PR China — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Münster 48149, Germany

At temperatures well below the glass transition temperature, the failure of metallic glasses is generally induced by shear-banding that is a result of the self-organized shear transformation zones (STZs). Here, we demonstrate that upon cooling down to liquid-helium temperature (4.2 K), a Zr-based metallic glass can fail via cavitation rather than by shear-banding due to the intervention of a ductile-to-brittle transition. This is supported by the breakdown of low-temperature strengthening of materials, as well as the change of fracture modes from shear to tension and fracture morphologies from vein-pattern to fine dimple or nanoscale periodic corrugation. We propose that a temperature-dependent STZ-dilatation, defined as the ratio of mobile free-volume to STZ-volume, controls the ductile-to-brittle transition, and across the transition point the STZ-type rearrangements of atomic-cluster will convert into the cavitation-dominated operations, i.e., tension transformation zones. Our findings shed new insight into fracture strength and energy dissipation mechanism in amorphous alloys, particularly at very low temperatures.

MM 22.2 Tue 10:30 IFW B

Microstructural influences on inhomogeneous plastic flow in AA2198 — ●HENRY OVRI and ERICA LILLEODDEN — Helmholtz Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Geesthacht, Germany

Inhomogeneous plastic flow has been reported in several Al alloys and is known to severely limit the formability of sheet metals and promote the formation of undesirable striations on the surface of the deforming part. Understanding the micromechanisms responsible for the occurrence of these plastic instabilities is pivotal to the design of alloys and process routes that mitigate the effect. Although it is widely accepted that the phenomenon is associated with dynamic strain aging (DSA) and negative strain rate sensitivity (NSRS), the effect of precipitation in retarding or enhancing the instabilities is still not clear. In this work, the effect of precipitation on inhomogeneous plastic flow in an Al-Li based alloy (AA2198) is investigated by using nanoindentation, atom probe microscopy and in situ TEM straining methods. The results are discussed on the basis of the observed interactions between matrix dislocations and coherent ordered δ' (Al₃Li) precipitates, residual matrix solute content and dislocation-particle interaction theories.

MM 22.3 Tue 10:45 IFW B

Tuning tensile ductility in composite structured Ti-based alloys — ●ILYA OKULOV^{1,2}, UTA KÜHN¹, JENS FREUDENBERGER^{1,3}, WERNER SKROTZKI⁴, and JÜRGEN ECKERT^{1,2} — ¹IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — ²Technische Universität Dresden, Institut für Werkstoffwissenschaft, D-01062 Dresden, Germany — ³Technische Universität Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Gustav-Zeuner- Str. 5, D-09599 Freiberg,

Germany — ⁴Technische Universität Dresden, Institut für Strukturphysik, D-01062 Dresden, Germany

Due to a well-balanced structure, Ti-based ultrafine-dendrite composites exhibit high strength and compressive plasticity already in the as-cast state. They consist of a β -Ti phase surrounded by ultrafine structured intermetallics: the β -Ti phase is ductile and tough one, while the brittle intermetallics effectively strengthen the alloys. The most of Ti-based ultrafine-dendrite composites are brittle in tensile loading. Recently, it was reported that the control of precipitates in the Ti-Nb-Cu-Ni-Al system can significantly enhance tensile ductility and maintaining high yield strength [1]. The approach was successfully applied to several Ti-based systems. And new composite structured alloys with high strength and tensile ductility were developed. For example, Ti68.8V13.6Cu6Ni5.1Al6.5 exhibits the ultimate strength of about 1250 MPa and the tensile ductility of about 4.5%.

1. Okulov et al. - Materials Science and Engineering C, 33 (2013) 4795-4801

MM 22.4 Tue 11:00 IFW B

Ab-initio modelling of mode I cleavage — ●BEATRIX A. M. ELSNER and STEFAN MÜLLER — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 HH

In this contribution we focus on the atomistic modelling of fracture, employing density functional theory to investigate the response of Cu and TiO₂ to mode I loading. As long as structural relaxations are omitted, the universal binding energy relation [1] may be applied to obtain the theoretical strength. However, relaxations can significantly affect the cleavage energy, and the stresses due to rigid displacement can only be considered an upper limit. If atomic relaxations are allowed, cleavage is treated as an energy minimization problem, and rupture will occur at the critical displacement l_c for which the Griffith criterion is fulfilled: $E_{\text{strain}}(l_c) = E_{\text{cleavage}}(l_c)$. As the strain energy depends on the system dimension perpendicular to the cleavage plane, the critical displacement is proportional to the square root of this system dimension. A consequence of this size effect are unphysical results in the limit of large system dimensions. We have used the nudged elastic band method (NEB) to study the transition from strain to cleavage, and we find that the energy barriers involved in the transition increase with increasing system size. This opposes the above-mentioned size effect and may limit the critical displacement. Further, our calculations suggest that prior to surface separation, the strain will localize close to the cleavage surfaces.

Supported by DFG, SFB 986, project B3.

[1] J. H. Rose, J. R. Smith, J. Ferrante, *Phys. Rev. B* **28**, 1835 (1983).

MM 22.5 Tue 11:15 IFW B

Residual stresses and internal architectures of AlSi-alloys for cast engine components — MICHAEL SCHÖBEL¹, GEORG BAUMGARTNER², and ●STEFAN GERTH³ — ¹Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), TU Munich, Germany — ²Umformtechnik und Gießereiwesen, TU Munich, Germany — ³Entwicklungszentrum für Röntgentechnik, Fraunhofer Institut Fürth, Germany

The increasing demand on weight and efficiency of modern combustion engines requires light alloys with improved high temperature strength and creep resistance. New cast AlSi alloys are developed to increase wear resistance and long term stability of engine components. In such materials with a composite-like micro structure high stress gradients lead to crack formation and damage under operation conditions.

Neutron diffraction is applied for micro stress analysis after casting as well as during tensile testing between the α -Al and Si phase. Complementary high resolution synchrotron tomography allowed 3D imaging of damage mechanisms and crack propagation. Both methods were combined to develop a micro-mechanical model for stress simulation and to validate its reliability for engineering AlSi alloys under reproducible boundary conditions.

MM 22.6 Tue 11:30 IFW B

In-situ Fatigue, Fracture and Dynamic Mechanical testing in the SEM — •DOUGLAS STAUFFER, SANJIT BHOWMICK, RYAN MAJOR, S.A. SYED ASIF, and ODEN WARREN — Hysitron, Inc. 9625 West 76th

St. Minneapolis MN

Rapid expansion of in situ nanomechanical testing gives researchers a means of testing and exploring fundamental deformation mechanisms. Here, new instrumentation involving novel control algorithms to control system quality factor is described, which allows the use of dynamic measurements without undesirable system oscillation. These dynamic measurements can then be used to explore frequency dependency, strain rate, fatigue, and crack propagation in a variety of materials. Here, frequency dependent effects are used to explore the effect of electron beam induced viscoplasticity in micron sized silica spheres. When tested without the presence of an electron beam, these spheres fracture at strains of less than 2%. However when irradiated at 20keV and 30pA in an SEM, the spheres can be deformed to strains of more than 50% under certain conditions. Rapid loading and high frequencies, correlated with high strain rates, result in fracture at strains of approximately 10% under e-beam irradiation. This is in contrast to slow loading and low frequency load controlled dynamic loading, where strains as large as 60% without fracture have been achieved.

MM 23: Electron Microscopy I - Nanomaterials

Time: Tuesday 10:15–11:30

Location: IFW D

MM 23.1 Tue 10:15 IFW D

Analytical EDX studies at different temperatures of Boron/Ni composite nanowires — •DANIELA SUDFELD, BASTIAN BARTON, OLEG LOURIE, and BERT FREITAG — FEI Electron Optics B. V., Eindhoven, The Netherlands

Analytical EDX studies at different temperatures were performed in a S/TEM, FEI Talos[TM] with ChemiSTEM[TM] Technology [1]. Fast chemical maps of B/Ni composite nanowires on nanometer scale by EDX (energy-dispersive X-ray spectroscopy) were done with the new Velox[TM] software. Successful synthesis of crystalline nanowires composed of the refractory light materials such as Boron can enable novel applications for nanoelectronics [2-4]. Boron/Nickel composite nanostructures were prepared by a CVD-based synthetic procedure with a Ni-based compound catalyst; naturally blended with high conductivity and refraction index. The properties of this binary nanomaterial at room temperature are compared to those achieved from heating experiments with temperatures up to 1000 deg C. 2D-3D EDX chemical mappings show clearly the core-shell structure of the wires: B in the shell and Ni in the core. This is amplified at elevated temperatures of ca. 500 deg C. At ca. 1,000 deg C EDX maps reveal also that Ni vanishes from the core, leaving behind hollow B nanowire (nanotube) structures. [1] P. Schlossmacher et al., *Microscopy Today* 18(4) (2010) 14. [2] CJ Otten, et al., *J Am Chem Soc.* 2002 May 1;124(17):4564. [3] D. Wang et al., *APL* 2003, 183(25):5280. [4] W. Ding et al., *Mech, Comp. Sci. and Techn.* 2006, 66:1109.

MM 23.2 Tue 10:30 IFW D

Evolution of the microstructure of amorphous FeNiP nanowire arrays upon in-situ annealing in TEM — •NINA WINKLER, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48149 Münster, Germany

In this work, an amorphous soft magnetic material is studied in confined dimensions regarding its crystallization behavior. Therefore, porous Anodic Alumina Oxide (AAO) is used because it enables the control of regularity and shape of nanostructures via its pores which are uniform in length and uniform in diameter. The fabrication of amorphous nanowire arrays by electrodeposition using AAO will be addressed. Upon in-situ annealing in the transmission electron microscope (TEM) the microstructural evolution could be monitored. Long range diffusion was observed following a phase separation of FeNiP in multilayers of FeNi and FeNiP phases. The impact of heating rates on the phase evolution is studied by controlled annealing with different heating rates of the FeNiP nanowires in atmosphere using a Differential Scanning Calorimeter (DSC). The magnetic properties of the nanowire arrays have been characterized with a Vibrating Sample Magnetometer (VSM). The results will be discussed with respect to the different microstructures of the nanowire arrays caused by the different thermal treatments.

MM 23.3 Tue 10:45 IFW D

Nucleation of embedded Pb nanoparticles in an Al(Ga) matrix — •ANNA MOROS¹, SORIN LAZAR², HARALD RÖSNER¹, PETER SCHLOSSMACHER², and GERHARD WILDE¹ — ¹Institute of Materials Physics, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — ²FEI Company, Achtseweg Noord 5, 5600 KA Eindhoven, The Netherlands

Undercooling of the liquid phase is often observed for most liquid pure materials. This indicates the existence of a large energy barrier to nucleate the solid phase. Heterogeneous nucleation at interfaces is generally favoured, since the nucleation barrier is reduced due to pre-existing catalytic substrates. Confined systems such as nanometer-sized particles embedded in a matrix have large specific interface areas that might possibly act as heterogeneous nucleation sites during solidification upon cooling, specifically since both, Pb and AlGa crystallize in fcc structure. In the present work, nanoscaled Pb inclusions embedded in AlGa matrices were processed by melt spinning technique. Various Ga quantities were alloyed into the matrix, since Ga is miscible with Al and immiscible with Pb. By means of differential scanning calorimetry, large undercoolings of Pb nanoparticles in (Al_{199-x}Ga_x)Pb₁ alloys were observed that increased with increasing amounts of Ga. At the same time, nanoscale chemical analyses using the SuperX detector implemented in a FEI Titan 60-300 microscope were performed and Ga segregation at the interfaces of the embedded Pb nanoparticles with AlGa-matrix was observed. In this contribution, the correlation between the segregation of Ga at the particle-matrix interface and the resulting undercooling of the nanoscaled Pb particles will be discussed.

MM 23.4 Tue 11:00 IFW D

Characteristics of shear bands in metallic glasses investigated by analytical TEM — •VITALIJ SCHMIDT, HARALD RÖSNER, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

In metallic glasses the entire deformation flow is restricted to narrow regions called shear bands. They are associated with a structural change compared to the surrounding matrix due to local distortion, most likely resulting in enhanced free volume. Therefore deformation properties of metallic glasses are determined by shear band characteristics which are a current object of research.

We present investigations of shear bands with a new approach that combines high angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) with electron energy loss spectroscopy (EELS) and energy dispersive x-ray (EDX) analysis. It is thereby possible to correlate dark-field intensity and local density by $\Delta\rho = \frac{I_{SB} - I_M}{I_M}$, where $\Delta\rho$ is the difference in density, I_{SB} and I_M are the HAADF intensities of the shear band and the matrix, respectively.

Cold-rolled Al₈₈Y₇Fe₅ melt-spun ribbons show shear bands having frequent contrast changes. Density measurements approve a continuous variation throughout the band* length implying different propagation velocities within the bright and dark parts.

MM 23.5 Tue 11:15 IFW D

Density of Grain Boundaries — •YULIA BURANOVA, SERGIY DIVINSKIY, HARALD RÖSNER, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

In this work we present the results of atomic simulations of different Grain Boundaries (GB) and the corresponding excess free volume defined as a relative density. For this purpose, an image analysis tool was designed that allows analyzing the local mass density on the basis of simulated (or experimental) high-resolution transmission electron microscopy (HRTEM) images. Thereto the intensities of the GB areas

were compared with that of the grain interiors and the difference was identified as the density change.

In total 24 different Symmetrical Tilt GB (STGB) were simulated. The density change in the STGB was estimated to be 5-6%. Experimentally, aluminum was investigated using HRTEM. Calculations showed that this method works for the pure samples with thicknesses up to 15nm including aluminum oxide layers. The correctness of the method is evaluated for different artificial configurations including chains of vacancies and solute atoms. The results and the method are discussed.

MM 24: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III (O with HL/TT/MM)

Time: Tuesday 10:30–13:15

Location: TRE Ma

Topical Talk MM 24.1 Tue 10:30 TRE Ma
Ultrafast relaxation dynamics of Hubbard nanoclusters — •MICHAEL BONITZ¹, SEBASTIAN HERMANN¹, CHRISTOPHER HINZ¹, and DENIS LACROIX² — ¹Institut für Theoretische Physik und Astrophysik, CAU Kiel, Leibnizstr. 15, 24098 Kiel — ²IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1]. The Hubbard model is a prototype for treating correlation effects in condensed matter or molecular systems fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system. In this talk we present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1] and, second, from a stochastic mean field approach.

[1] K. Balzer, and M. Bonitz, “Nonequilibrium Green’s Functions Approach to Inhomogeneous Systems”, *Lect. Notes Phys.* **867** (2013)

MM 24.2 Tue 11:00 TRE Ma
Exact adiabatic approximation in TDDFT — •JEIRAN JOKAR and NICOLE HELBIG — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The use of functionals from static density functional theory in an adiabatic way in a time-dependent framework is known to cause various problems due to the resulting exchange-correlation kernel being frequency independent. In order to isolate the effects which are due to the adiabatic approximation we calculate the exact static potential for two electron systems. Before using this potential in an adiabatic way in a time propagation we need to ensure that the potential is well defined also at those parts of space where the density is small as they might become more populated at a later time. We use the exact adiabatic approximation to describe Rabi oscillations, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied.

MM 24.3 Tue 11:15 TRE Ma
Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems — •RENÉ JESTÄDT¹, HEIKO APPEL¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Based on the Riemann-Silberstein vector of the electromagnetic field, we formulate Maxwell’s equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques developed for the Schrödinger equation [1] also for Maxwell’s equations and simplifies a coupled solution of Maxwell’s and Schrödinger’s equations. To il-

lustrate our approach, we present the real-time evolution of atomic systems embedded in optical waveguides and dielectric nanostructures. The coupling of Maxwell’s equations to the time-dependent Kohn-Sham equations is a basic ingredient for the development of a time-dependent density functional theory formulation of quantum electrodynamics [2]. As an extension of our work on coupled Maxwell-Schrödinger systems, we show first steps of an implementation of Maxwell’s equations coupled to the time-dependent Kohn-Sham equations in the first principles real-space real-time code octopus [3].

[1] A. Castro et al., *J. Chem. Phys.* **121** (2004).

[2] M. Ruggenthaler, F. Mackenroth, and D. Bauer, *Phys. Rev. A* **84**, 042107 (2011); I. Tolkatly, *Phys. Rev. Lett.* **110**, 233001 (2013).

[3] X. Andrade et al., *J. Phys. Cond. Mat.* **24** (2012).

MM 24.4 Tue 11:30 TRE Ma
Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation — •CLAUDIO ATTACCALITE¹ and MYRTA GRUNING² — ¹Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — ²School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, Northern Ireland, UK

We present an real-time approach to study nonlinear optical properties in Condensed Matter systems that is especially suitable for crystalline solids. The equation of motions and the coupling of the electrons with the external electric field are derived from the Berry phase formulation of the dynamical polarization. Many-body effects are introduced by adding single-particle operators to the independent-particle Hamiltonian. Specifically we include crystal local field effects, renormalization of the energy levels and excitonic effects. The approach is validated by calculating the second and third harmonic generation of bulk semiconductors. Finally we present second-harmonic generation spectrum of h-BN or MoS2 monolayers and show that correlation effects double the signal intensity at the excitonic resonances with respect to the contribution from independent electronic transitions.

References: [1] Nonlinear optics from ab-initio by means of the dynamical Berry-phase <http://arxiv.org/abs/1309.4012> [2] Second Harmonic Generation in h-BN and MoS2 monolayers: the role of electron-hole interaction <http://arxiv.org/abs/1310.7459>

15 min. break

MM 24.5 Tue 12:00 TRE Ma
Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels — •THOMAS OLSEN¹ and KRISTIAN S. THYGESEN² — ¹Universidad del País Vasco — ²Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

We demonstrate the accuracy of electronic correlation energies obtained from the adiabatic connection and Time-Dependent Density Functional Theory (TDDFT) using a non-empirical renormalized gradient-corrected exchange-correlation kernel. The method can be viewed as a natural step beyond the Random Phase Approximation (RPA) and captures the short-range correlation effects which are poorly described in RPA. In particular, we show that for molecules and solids the renormalized kernel gives a four and five fold improvement in binding energies respectively when compared to RPA. We also consider examples of barrier heights in chemical reactions, molecular adsorption and graphene interacting with metal surfaces, which are

three examples where RPA has provided highly accurate results. In these cases, our novel kernel provides results that are of equal quality or even slightly better than RPA, with a similar computational cost. We finally note that the renormalization procedure can be applied to any known semi-local exchange-correlation functional and thus defines an entire new class of adiabatic non-local functionals for ground state calculations within TDDFT.

MM 24.6 Tue 12:15 TRE Ma

Low scaling algorithm for the random phase approximation — ●MERZUK KALTAK, JIRI KLIMEŠ, and GEORG KRESSE — University of Vienna, Computational Material Physics

The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability χ . We present an RPA algorithm that calculates χ using the Green function G in real space and imaginary time. The systematic construction of optimized time and frequency grids for G is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPA correlation energy for large systems.

MM 24.7 Tue 12:30 TRE Ma

Long range correlation energy from coupled atomic response functions — ●ALBERTO AMBROSETTI and ALEXANDRE TKATCHENKO — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Germany

Electron correlation is an elusive and ubiquitous energy contribution that arises from transient collective electron fluctuations. Its reliable (accurate and efficient) modeling is central to the correct description of cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose a very efficient method to compute the long-range correlation energy for non-metallic molecules and solids within a density functional theory framework, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing for a seamless many-body treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), large supramolecular complexes (S12L), molecular crystals (X23) and bulk graphite shows consistently good agreement with high level theoretical and experimental reference binding energies (within the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

MM 24.8 Tue 12:45 TRE Ma

The exact Hohenberg-Kohn functional for a lattice model —

●TANJA DIMITROV¹, HEIKO APPEL¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals and to gain insight into the behavior of the exact functional, we investigate the exact solution of the many-body Schrödinger equation for a lattice model. Using exact diagonalization, we explicitly construct the exact Hohenberg-Kohn functional and the mapping from densities to wavefunctions. Besides the normal inter-system derivative discontinuity widely discussed in the density-functional theory community, we observe a new feature of the exact functional in the low-density limit. This "intra-system derivative discontinuity" resembles the inter-system derivative discontinuity, but is within the system (work in progress [3]). The description of many physical phenomena linked to charge-transfer processes (both in the static and dynamical regimes) require a proper account of this "intra-system derivative discontinuity".

[1] A. J. Cohen et al. Science **321**, 792 (2008).

[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).

[3] T. Dimitrov, H. Appel, A. Rubio to be published

MM 24.9 Tue 13:00 TRE Ma

Incorporating static correlation effects into density functional theory — NEKTARIOS N. LATHIOTAKIS¹, ●NICOLE HELBIG², NIKITAS I. GIDOPOULOS³, and ANGEL RUBIO^{4,5} — ¹Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — ²Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — ³Department of Physics, Durham University, United Kingdom — ⁴Nano-Bio Spectroscopy group, Universidad del País Vasco and DIPC, San Sebastian, Spain — ⁵Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a novel idea that builds on the knowledge acquired in Reduced density matrix functional theory (RDMFT) to construct a density-functional scheme which accurately incorporates static and left-right correlation effects. At the same time, the new scheme preserves the high quality of a density functional description at the equilibrium and keeps the computational costs at an acceptable level comparable to the costs when using hybrid functionals. Within this scheme the natural orbitals, i.e. the eigenfunctions of the one-body density matrix, are constrained to be solutions of a single-particle Schrödinger equation with a local effective potential. This provides a natural way to connect an energy eigenvalue spectrum to the natural orbitals. This energy spectrum is found to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit of diatomic molecules is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved. The present scheme can be easily implemented in all first principles codes for electronic structure calculations.

MM 25: Topical Session: Thermodynamics at the nano scale II - Thermodynamics

Time: Tuesday 11:45–13:00

Location: BAR 205

Topical Talk

MM 25.1 Tue 11:45 BAR 205

Metal-hydrogen (M-H) systems: a tool for studying changes of thermodynamics and kinetics due to size reduction — ●ASTRID PUNDT — Institut für Materialphysik, Universität Göttingen, Göttingen, Germany

Hydrogen easily solves on interstitial lattice sites in metals. Its high diffusivity results in short alloying times even at room temperature. At 300 K, the intrinsic defect density and the sample shape remains rather stable. This enables us to study thermodynamical and kinetical changes related to size reduction of the metal.

Many size-related effects have been reported during the last years. They are often generated by a mixture of effects due to sample size, micro-structure and mechanical stress contributions.[1] Challenge here is to split those effects related to the size reduction (finite-size effects) from those related to micro-structural changes and the mechanical stress that arises between the sample and the required stabilizer. For this, M-H thin films and M-H clusters serve as model systems. It

will be shown that for systems of about 30 nm and larger the classical thermodynamics holds and conventional stress release occurs while for smaller system sizes coherent thermodynamics comes into play and ultra-high stresses are found.

Financial support by the DFG is gratefully acknowledged.

[1] A. Pundt, R. Kirchheim, Ann. Rev. Mat. Res. **36** (2006) 555.

MM 25.2 Tue 12:15 BAR 205

Ab initio study of AlN: thermodynamic properties, phase diagram and high temperature rock salt to wurtzite phase transition — ●STEVE SCHMERLER and JENS KORTUS — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

We review our recent work [1] on AlN regarding the wurtzite – rock salt phase boundary calculated within the quasiharmonic approximation by using density functional perturbation theory. We discuss exchange-correlation functional effects on the phase boundary and other thermodynamic properties. Additionally, we present *ab initio* molecular

dynamics results regarding a temperature-driven rock salt to wurtzite backward phase transition and propose a detailed transition mechanism.

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

[1] M. Schwarz, M. Antlauf, S. Schmerler, K. Keller, T. Schlothauer, J. Kortus, G. Heide and E. Kroke, High Pressure Res. (2013), dx.doi.org/10.1080/08957959.2013.857020

MM 25.3 Tue 12:30 BAR 205

Concept of multicomponent alloying based on self-organization on the nanoscale. — ●IGOR A. ABRIKOSOV — IFM, Linköping University, Sweden

We propose a design route for the next generation of nitride alloys via a concept of multicomponent alloying based on self-organization on the nanoscale via a formation of metastable intermediate products during the spinodal decomposition. Experimentally the formation of detrimental wurtzite AlN phase has been identified as a major factor limiting the thermal stability of the state-of-the-art (TiAl)N alloys used in modern hard coating applications. We carry out systematic first-principles calculations aimed at finding potential new multicomponent transition-metal aluminum nitride alloys, and identify Cr as one of the most promising alloying elements. We predict theoretically and demonstrate experimentally that quasi-ternary (TiCrAl)N alloys decompose spinodally into (TiCr)N and (CrAl)N-rich nanometer sized regions. The spinodal decomposition results in age hardening, while

the presence of Cr within the AlN phase delays the formation of a detrimental wurtzite phase leading to a substantial improvement of thermal stability compared to the quasi-binary (TiAl)N or (CrAl)N alloys [1].

[1] H. Lind, R. Forsen, B. Alling, N. Ghafoor, F. Tasnadi, M. P. Johansson, I. A. Abrikosov, and M. Oden, Appl. Phys. Lett. 99, 091903 (2011); H Lind, F Tasnadi and I A Abrikosov, New J. Phys. 15 095010 (2013)

MM 25.4 Tue 12:45 BAR 205

Reversible Phase transition of Li₁₃Si₄ — ●THOMAS GRUBER and JENS KORTUS — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

Li_xSi seems to be a promising new anode material for lithium ion batteries. For any proper application the calculation of thermodynamical data like the specific heat is required to understand the behavior of this material. There are several crystalline phase of the lithium-silicon system known and the Li₁₃Si₄ phase is somehow special. The phonon calculation reveal some imaginary frequencies and our evolutionary algorithm “EVO” [1] found a new similar structure. Nudged Elastic Band (NEB) method and molecular dynamic (MD) calculations were used to get a deeper insight into the phase transition between these two structures with a very low activation barrier. A very fast 1 dimensional lithium diffusion has been observed, which is very important for electrode material.

[1] S. Bahmann, J. Kortus, Computer Physics Communications 2013, 184, 1618-1625.

MM 26: Computational Materials Modelling IV - Phase transitions II

Time: Tuesday 11:45–13:00

Location: IFW D

MM 26.1 Tue 11:45 IFW D

Study of the austenite-martensite phase transition in steel using molecular dynamics — ●EMILIA SAK-SARACINO and HERBERT M. URBASSEK — Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern

Using molecular-dynamics simulation, we study the austenite-martensite phase transition in various iron alloys. In these, we consider a dilute mixture of the alloying element (C, Ni or Cu) up to 1 at-%. The specimens are subjected to a heating/cooling cycle. The phase transition can be observed by monitoring the hysteresis of the system volume with temperature. For the alloying elements studied, we find that martensite and austenite temperatures decrease with increasing concentration, in agreement with experiment.

MM 26.2 Tue 12:00 IFW D

Atomistic simulations of solid-solid phase transformations in molybdenum — ●ARI HARJUNMAA¹, JUTTA ROGAL¹, RALF DRAUTZ¹, RYE TERRELL², SAM CHILL², and GRAEME HENKELMAN² — ¹ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²Department of Chemistry and the Institute for Computational and Engineering Sciences, University of Texas at Austin, Austin, Texas 78712, USA

As a refractory metal, molybdenum plays an important role in strengthening special-purpose materials such as Ni-base superalloys. In heavy usage, these materials are frequently plagued by the formation of topologically close-packed (TCP) phases, which concentrate the alloying atoms into brittle precipitates, rendering the material weaker. To find a way to prevent this detrimental occurrence, it is important to understand the atomistic processes at work in solid-solid phase transformations leading to the formation of TCP phases. As a first step, we investigate interfaces between the TCP A15 and the cubic BCC phases in molybdenum, using classical molecular dynamics to model the time evolution of the systems in question. We then compare and expand these results with those obtained from adaptive kinetic Monte Carlo simulations, extending the same system setup to room temperature; furthermore, we use this latter method to characterize singular processes involved in the transformation of the atomic layers. Finally, we evaluate the reliability of the employed empirical potential by further analysis of the main results using density functional theory.

MM 26.3 Tue 12:15 IFW D

Importance of anharmonic free energy contributions in an *ab initio* description of the hcp to bcc transition in Ti — ●DOMINIQUE KORBMACHER, ALBERT GLENSK, BLAZEJ GRABOWSKI, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti and its alloys are a very important class of materials with various technical and medical applications. Further optimizing the properties of these alloys requires accurate and reliable phase diagrams. A recent and very promising approach is the construction of phase diagrams based on finite temperature *ab initio* simulations [1]. However, a critical and so far unresolved difficulty when dealing with Ti based systems is the dynamical instability of the Ti bcc phase at $T=0$ K.

In the present study, we investigate the hcp to bcc phase transition in Ti including the anharmonic contribution on a fully *ab initio* basis (density-functional theory). To overcome the long CPU simulation times typically involved in calculating anharmonicity, we use here the recently developed UP-TILD method [1]. We show that the low temperature hcp phase is well described when comparing with experimental data (e.g., heat capacity). For the high temperature bcc phase the dynamical stabilization due to phonon-phonon interaction is correctly predicted, but we show that the commonly used exchange-correlation functional (GGA-PBE) yields a too soft expansion and a too low phase transition temperature. We discuss whether alternative xc-functionals can improve the situation.

[1] B. Grabowski, et al., PRB **79**, 134106 (2009).

MM 26.4 Tue 12:30 IFW D

Simulating Order Parameters for Phase Transitions in Alloys — ●CONRAD W. ROSENBRUCK, GUS L. W. HART, BRANTON J. CAMPBELL, and RICHARD R. VANFLEET — Brigham Young University, Provo, UT, 84602, USA

When determining the structure of alloys using diffraction patterns, possible distortions that lower the symmetry of the parent phase can be limited by group-theoretical arguments as long as a group-subgroup relationship exists between the parent and distorted phases¹. Order parameters are vectors in representation space where each dimension corresponds to a specific superlattice vector in reciprocal space (e.g. $L = [0.5, 0.5, 0.5]$ or $X = [1, 0, 0]$); such order parameters determine the distortions that may arise during a phase transition. By measuring the Fourier transform of the structure at each relevant superlattice vector during a Monte Carlo simulation for CuPt₃, we were able to ex-

tract these thermodynamic order parameters and qualitatively confirm distortions in the L and X order parameters observed in experiment². The methodology presents a highly effective avenue for comparing simulated phase transitions with experimental results.

[1] Harold T. Stokes, Branton J. Campbell and Dorian M. Hatch. *Order parameters for phase transitions to structures with one-dimensional incommensurate modulations*

[2] Rokuro Miida and Denjiro Watanabe. *Electron Microscope and Diffraction Study on the Ordered Structures of Platinum-Rich Copper-Platinum Alloys*

MM 26.5 Tue 12:45 IFW D

Phase-field simulation of the peritectic reaction in Al-Cu-Ni

MM 27: Transport I - Materials/Methods

Time: Tuesday 11:45–13:00

Location: IFW B

MM 27.1 Tue 11:45 IFW B

Studying spatially resolved atomic diffusion processes using X-rays - atomic-scale X-ray photon correlation spectroscopy and its application to metallic alloys — ●MARKUS STANA¹, MICHAEL LEINTNER², MANUEL ROSS¹, and BOGDAN SEPIOL¹ — ¹Universität Wien, Fakultät für Physik, Boltzmannngasse 5, 1090 Wien, Austria — ²Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85747 Garching, Germany

In the recent years our group succeeded in studying spatially resolved diffusion processes on the atomic scale by extending X-ray photon correlation spectroscopy (XPCS) to large scattering angles. In my talk I will give an overview of this new technique and present the results we achieved for binary metallic systems. Special attention will be given to solid solutions (Ni-Pt) and intermetallic phases like B2 (Fe-Al) and L1₂ (Cu-Au, Ni-Pt). I will conclude by briefly showing that this technique can also shed light on atomic motion in noncrystalline systems like glasses.

This work was financially supported by the Austrian Science Fund (FWF) P-22402.

MM 27.2 Tue 12:00 IFW B

Diffusion of Atoms and Vacancies in Thin Nano Crystalline Platinum Films — ●WOLFGANG GRUBER¹, JOHANNA RAHN¹, FLORIAN STRAUSS¹, LARS DÖRRER¹, ERWIN HÜGER¹, MICHAEL HORISBERGER², THOMAS GEUE², JOCHEN STAHN², CARSTEN BÄHTZ³, WOLFRAM LEITENBERGER⁴, and HARALD SCHMIDT¹ — ¹TU Clausthal — ²Paul Scherrer Institut — ³Helmholtz-Zentrum Dresden-Rossendorf — ⁴Universität Potsdam

An important characteristic of thin metal films deposited on substrates is the presence of a high number of defects in the metal film which is correlated to residual stress and strain. During heat treatment strain in the metal films relaxes. The relative changes of the film thickness and the interplanar distance are correlated to the change of the defect concentration during relaxation. In-situ X-ray diffraction and X-ray reflectometry using synchrotron radiation revealed that strain relaxation is accompanied by an increase of the vacancy concentration at the surface of the film [1]. In this work we present experimental results supporting the stress relaxation model outlined in [1]. To clarify the rate determining process for strain relaxation, grain boundary and volume self-diffusion of platinum is investigated. Samples enriched in the stable isotope ¹⁹⁴Pt as tracer source were prepared and used for analysis with secondary ion mass spectrometry and neutron reflectometry. [1] W. Gruber, S. Chakravarty, C. Baecht, W. Leitenberger, M. Bruns, A. Kobler, C. Kübel, H. Schmidt, Phys. Rev. Lett. 117 (2011) 265501.

MM 27.3 Tue 12:15 IFW B

Conductance through itinerant geometrically frustrated electronic systems — ●ALEXANDRE LOPES¹, BRUNO ANTÓNIO², and RICARDO DIAS² — ¹Institute of Physics, University of Freiburg, Herman-Herder-Straße 3, 79104 Freiburg, Germany — ²Universidade de Aveiro, I3N, Campus Universitário de Santiago, Aveiro, Portugal

We study a two terminal electronic conductance through an AB₂ ring which is an example of the family of itinerant geometrically frustrated

alloys — ●JULIA KUNDIN, HEIKE EMMERICH, and EVGENY POGORELOV — University Bayreuth

The simulations of the solidification of ternary Al-Cu-Ni alloys were carried out by means of a general multi-phase-field model for an arbitrary number of phases. A realistic microstructure can be generated by coupling the real thermodynamic parameters of the phases and the evolution equations. The stability requirements for the model functions on every dual interface guarantee the absence of "ghost" phases on them. The thermal noise terms disturb the stability and can produce the heterogeneous nucleation of product phases in accordance to the energetic conditions. It is shown that the model can produce the growth of the combined eutectic-like and peritectic-like structure in various alloys. Of particular interest is the heterogeneous nucleation of the fourth phase in triple points.

electronic systems. These systems are characterized by the existence of localized states with nodes in the probability density. We show that such states lead to distinct features in the conductance. For zero magnetic flux, the localized states act as a filter of the zero frequency conductance peak, if the contact sites have hopping probability to sites which are not nodes of the localized states. For finite flux, and in a chosen orthonormal basis, the localized states have extensions ranging from two unit cells to the complete ring, except for very particular values of magnetic flux. The conductance exhibits a zero frequency peak with a dip which is a distinct fingerprint of the variable extension of these localized states.

MM 27.4 Tue 12:30 IFW B

Conductivity and Dielectric Properties of Li_xNa_{2-x}Ti₆O₁₃ (x = 0...2) — ●KAI VOLGMANN and PAUL HEITJANS — Leibniz Universität Hannover, Inst. f. Phys. Chemie u. Elektrochemie, Callinstr. 3 - 3a, D-30167 Hannover

Titanate systems attract much attention as anode material for secondary Li ion batteries due to advantages compared to graphite. TiO₂ is a prominent example within the system Li₂O - TiO₂. In the present work, Li_xNa_{2-x}Ti₆O₁₃ (space group C2/m) has been chosen as a model system because of its channel-like crystal structure. The alkali atoms are solely located inside the channels. The samples with different Li/Na ratios were characterized by powder x-ray diffraction and inductively coupled plasma optical emission spectroscopy (ICP-OES). Impedance spectroscopy measurements were performed over a wide temperature range (200-1000 K). Thin films of graphite or Pt were used as electrodes. The frequency dependent conductivity data yielded activation energies E_A which partly depend on the Li/Na ratio. Whereas E_A values calculated from the DC plateau are essentially independent of x, the AC contribution has a maximum E_A value for x = 0.33. Cole-Cole plots of the complex impedance show a depressed semicircle. Thus no separation of bulk and grain boundary contributions is visible. Plotting the complex modulus vs. frequency shows different relaxation modes corresponding to different bulk processes. Comparison of the various representations gives information on the diffusivity of the alkali ions on macroscopic and microscopic scales.

MM 27.5 Tue 12:45 IFW B

Short Range Silicon Migration in Amorphous Silicon Observed by Neutron Reflectometry — ●FLORIAN STRAUSS¹, HARALD SCHMIDT¹, JOCHEN STAHN², and THOMAS GEUE² — ¹TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — ²Paul Scherrer Institut, Villigen, Schweiz

Amorphous silicon (a-Si) is a simple model system of covalent amorphous semiconductors, widely used in solar cells and flat screen displays and a promising electrode material in Li-ion batteries. Yet, there exist no experimental data on self-diffusion in the amorphous state. The expected low diffusivities and intrinsic metastability of a-Si require measurement by time-of-flight neutron reflectometry (NR), a method capable of determining diffusion lengths of 1 nm and below [1,2]. ²⁹Si/²⁸Si isotope multilayers are prepared by ion beam sputtering and thermally treated in Ar atmosphere at temperatures below the crystallisation temperature in order to induce interdiffusion. The samples are isotope modulated but amorphous and chemically homogenous

as shown by TEM and XRD. Previous measurements have pointed to an onset of movement above 350 °C and short range atomic diffusion processes on the length scale of 1.5 - 2 nm. New data from NR and SIMS are discussed, focussing on time dependent diffusion processes and long range motion at temperatures between 400 °C and 600 °C.

The influence of impurities on diffusion and structure is also part of the on-going investigation.

[1] H. Schmidt et al.; *Acta Mater.* 56 (2008), 464

[2] E. Hüger et al., *Appl. Phys. Lett.* 93 (2008), 162104

MM 28: Nanomaterials I - Synthesis of advanced nanostructures

Time: Tuesday 12:00–13:15

Location: IFW A

MM 28.1 Tue 12:00 IFW A

An apparatus for the synthesis of cluster-based materials — ●ARNE FISCHER, ROBERT KRUK, and HORST HAHN — Karlsruhe Institut für Technologie, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany

A cluster deposition system for the synthesis of materials composed of mass-selected clusters embedded in various matrices as well as cluster-decorated surfaces was constructed and first deposition experiments were performed.

The system covers a large range of cluster sizes from single atoms up to clusters consisting of several thousands of atoms and provides a cluster beam with a narrow size distribution. Offering the ability to co-deposit matrix materials and mass selected clusters in well-defined ratios the system allows for studying material properties as a function of cluster size and density in the matrix. Hence this approach can open pathways to a new class of materials with tailored electronic, magnetic or catalytic properties.

In recent experiments the exchange bias was studied in thin films composed of ferromagnetic clusters and antiferromagnetic matrix materials.

MM 28.2 Tue 12:15 IFW A

Micro and nano-scale magnetic structures created by electron beam induced deposition — JOHANNES J.L. MULDER and ●DANIELA SUDFELD — FEI Electron Optics B. V., Eindhoven, The Netherlands

Electron beam induced deposition is a direct write patterning technique, using the electron beam of a scanning electron microscope (SEM) to locally dissociate injected precursor molecules adhered to a surface[1]. This dissociation results in a split of the precursor molecule into a volatile part (such as Fe) and a non-volatile part (such as CO), that is pumped out. The non-volatile part forms a deposit at the location of the electron beam and because the lateral patterning is done with nano-scale accuracy and the vertical growth is controlled by the dwell time, the technique offers a direct write patterning capability in 3 dimensions. Recently the material quality of the actual deposition of magnetic materials such as Co and Fe, has reached a level allowing for the creation of nano-scale magnetic structures that can be used for domain wall pinning, Hall sensors, and tips for magnetic force microscopy (MFM). The current status of the technology will be presented, including the practical limits and recent examples. In addition results using Co and Fe precursors, as well as a brief outlook into the near future will be presented. [1] Botman A., Mulders JJL, Hagen CW, *Nanotechnology* 20 (2009) 372001

MM 28.3 Tue 12:30 IFW A

Optical printing of gold nano resonators — ●ANDREAS GRAW, SPAS NEDEV, THEOBALD LOHMÜLLER, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80799 München, Germany

Plasmonic coupling between two closely apposed gold nanoparticles leads to a strong enhancement of the electromagnetic field in the nanoparticle gap. Such strongly coupled nanostructures, or plasmonic nanoantennas, offer outstanding capabilities for label-free sens-

ing, spectroscopy, and optical manipulation at the nanoscale [1].

However, the exact positioning of individual nanoparticles right next to each other is challenging and requires high-end nanofabrication methods such as eBeam lithography or manipulation with an AFM tip. Here, we introduce an all optical approach to pattern gold nanoparticles with nanoscale accuracy by optical forces [2]. In this context, we will demonstrate how individual gold particles can be printed on a glass substrate with light and discuss strategies to apply this approach for the fabrication of plasmonic nanoantennas.

[1] Ringler, M.; *Nano Lett.* 2008, 8(2), 485-490

[2] Urban, A; *Nano Lett.* 2010, 10(12), 4794-4798

MM 28.4 Tue 12:45 IFW A

Multiple scribing via diffusion-assisted direct laser writing — ●IOANNA SAKELLARI¹, JAE-HYUCK YOO², DAVID GRAY³, MARIA VAMVAKAKI³, NIKITA BITYURIN⁴, ALEXANDER PIKULIN⁴, COSTAS GRIGOROPOULOS², and MARIA FARSARI³ — ¹University of Stuttgart, Stuttgart, Germany — ²University of California, Berkeley, USA — ³Institute of Electronic Structure and Laser, Heraklion, Greece — ⁴Russian Academy of Sciences, Nizhni Novgorod, Russia

Direct Laser Writing by Two-Photon Polymerization is a versatile technique for the creation of solid 3D polymer nanostructures for photonics, biomedical and microfluidic applications. By employing laser intensities that are only slightly above the nonlinear polymerization threshold, structures with resolution of 100nm can be fabricated. In this work, we report our recent results on resolution improvement of DLW by exploiting the diffusion of a mobile quenching molecule in the scanned area. By employing a multiple scribing method, we exploit the resulted depletion of the multi-photon generated radicals in between the scans allowing the fabrication of high resolution structures. The material used is an organic-inorganic hybrid composite containing a zirconium based hybrid, while the quencher used is also a photopolymerizable monomer that becomes part of the polymer backbone upon fabrication. 3D woodpile structures with lateral spatial resolution of 70nm and rod spacing of 300nm are successfully fabricated. Optical characterization of the fabricated structures clearly shows that they exhibit stop gaps down to visible wavelengths, while well-ordered diffraction patterns obtained reveal high quality samples.

MM 28.5 Tue 13:00 IFW A

Thermal Curing of Polymers at the Nanoscale by Optothermal Manipulation of Gold Nanoparticles — ●JAKOB LENZ, CHRISTOPH MAIER, MICHAEL FEDORUK, THEO LOHMÜLLER, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Amalienstraße 54, München

Light absorbed by small gold nanoparticles is very efficiently converted into heat on a picosecond timescale. Single particles can thus be used as a heat source on a very confined, nanoscopic area. Here we demonstrate how these properties can be utilized to trigger and control the heat induced polymerization reaction of thermosetting polymers at the nanoscale and show how this approach can be applied to fabricate polymer nanostructures such as particles and nanowires with a resolution well below the diffraction limit. Overall, this approach represents a new way of controlling polymerization reactions at the nanoscale by taking advantage of plasmonic heating.

MM 29: Invited Talk (Hauptvortrag) Divinski

Time: Tuesday 15:00–15:30

Location: BAR 205

Invited Talk

MM 29.1 Tue 15:00 BAR 205

Grain boundaries in metals: phase and structure transitions studied by tracer diffusion — ●SERGIY DIVINSKI — Institut für Materialphysik, Universität Münster

Recent advances in measurement techniques have allowed extending the radiotracer experiments on grain boundary diffusion of solutes in bicrystals to substantially lower temperatures. As a result, the data on grain boundary diffusion coefficients and those of the product of the solute segregation and the grain boundary width were independently evaluated and compared with the polycrystalline data [1]. The segregation of Ag at Cu $\Sigma 5$ and $\Sigma 17$ grain boundaries is found to be significantly stronger as compared to that at general high-angle grain boundaries as they are present in annealed polycrystalline copper. The

grain boundary diffusion data predict a structural transition in the $\Sigma 5$ grain boundary at a temperature of about 850 K what was recently confirmed by dedicated MD simulations [2]. Strong solute segregation could induce grain boundary phase transitions, too. An abrupt increase of the grain boundary diffusivity was observed in a two-phase (solid+liquid) region of the Cu-Bi phase diagram [3]. Such diffusion enhancement exists even in a single phase (solid solution in Cu) region manifesting the existence of a pre-wetting GB phase transition in this system. These and other findings with respect to short-circuit diffusion in bi- and tri-crystals are reviewed and critically discussed.

[1] S.V. Divinski, et al. Phys Rev B 85 (2012) 144104.

[2] T. Frolov, et al. Phys Rev Lett 110 (2013) 255502.

[3] S.V. Divinski, et al. Phys Rev B 71 (2005) 104.

MM 30: Topical Session: Thermodynamics at the nano scale III - Novel experimental and theoretical approaches

Time: Tuesday 15:45–17:45

Location: BAR 205

MM 30.1 Tue 15:45 BAR 205

Efficient evaluation of thermoelectric and electronic transport properties in a maximally-localized Wannier-function basis using the BoltzWann code — ●GIOVANNI PIZZI¹, DMITRI VOLJA², BORIS KOZINSKY³, MARCO FORNARI⁴, and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials, EPFL (CH) — ²Department of Materials Science and Engineering, MIT (USA) — ³Robert Bosch LCC Research and Technology Center, Cambridge (USA) — ⁴Dept. of Physics, Central Michigan University (USA)

The calculation of thermoelectric and electronic transport properties of extended systems requires extremely dense Brillouin-zone samplings together with the evaluation of band derivatives, that are however difficult to converge using standard finite-difference methods in systems where band crossings are present. We address both issues in our BOLTZWANN code [1] by adopting a maximally-localized Wannier function basis set. This allows both to interpolate the bands with very high accuracy thanks to the strong localization of the Wannier functions, and to calculate band derivatives analytically giving precise results also in the case of band crossings. BOLTZWANN then solves the semiclassical Boltzmann transport equations in the constant relaxation-time approximation to obtain transport properties (conductivities, Seebeck coefficient). We apply the code to some relevant systems like the CoSb₃ and CoGe_{3/2}S_{3/2} skutterudites. BOLTZWANN is freely distributed as a module within the Wannier90 2.0 code [2].

[1] G. Pizzi *et al.*, Comp. Phys. Comm. 185, 422 (2014)

[2] www.wannier.org

MM 30.2 Tue 16:00 BAR 205

Gaussian Approximation Potential: an interatomic potential derived from first principles Quantum Mechanics — ●ALBERT BARTÓK-PÁRTAY and GÁBOR CSÁNYI — Department of Engineering, University of Cambridge, Trumpington Street, CB21PZ, Cambridge, UK

We present a method that allows the exploration of the DFT Born-Oppenheimer potential energy surface by interpolating between pre-computed values at a set of points in atomic configuration space. The resulting model does not have a fixed functional form and hence is capable of modelling complex potential energy landscapes. In order to achieve this, we developed an invariant representation of the atomic environment. The potential is systematically improvable with more data. The accuracy of this interpolated PES is remarkable for a wide variety of systems, including semiconductors, metals and polarisable crystals.

MM 30.3 Tue 16:15 BAR 205

Ab initio prediction of solvus lines in Al alloys: The importance of anharmonic contributions — ●ALBERT GLENSK, BLAZEJ GRABOWSKI, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf

The prediction of alloy phase diagrams without any experimental in-

put is a major challenge in materials science. First-principles studies including temperature effects in the harmonic approximation have already demonstrated to provide a qualitative agreement with CALPHAD phase diagrams, but truly quantitative predictions are rare. Recent first-principles calculations on point defects have shown that a highly accurate computation of formation free energies is possible up to the melting temperature, if all excitation mechanisms, in particular anharmonic excitations, are taken into account [1]. Applying these methods, we have studied the solvus line of Si in Al, giving access to the Al-rich region of the Al-Si phase diagram. We will discuss the methodological challenges and the unexpectedly large impact of anharmonic lattice excitation on these results.

[1] B. Grabowski et al, PRB 79, 134106 (2009)

MM 30.4 Tue 16:30 BAR 205

Low temperature specific heat of pure titanium made nanocrystalline by severe plastic deformation — ●MARTIN PETERLECHNER¹, JOCHEN FIEBIG², and GERHARD WILDE¹ — ¹Institute of materials physics, WWU Münster, Germany — ²Department of Chemical Engineering and Materials Science, UC Davis, USA

In the last decades it was shown that severe plastic deformation can be used to obtain bulk nanostructured materials. In the present work, pure titanium was processed by equal channel angular pressing and subsequently annealed to obtain fairly dislocation free bulk nanostructured samples. The arising structures were analyzed using electron microscopy. Specific heat measurements using the two-tau method were conducted in the temperature range between 1.9 and 300 K, to obtain data sets of nanocrystalline titanium and its coarse grained counterpart. Using the Debye model for the lattice-vibrational contribution to the low temperature specific heat (<5K), and using the Sommerfeld model for the contribution of the electrons to the specific heat a function $g^*T+a^*T^3$ was fitted to obtain the Sommerfeld coefficient g and the Debye temperature. It is concluded, that in nanocrystalline titanium the contribution of electrons to the specific heat is increased due to the high number of grain boundaries. There is an indication that the Debye temperature slightly decreases and, moreover, the total enthalpy of the nanocrystalline phase increases. Based on the results thermodynamic properties of grain boundaries are deduced, and the limits of the applied models are discussed.

15 min break**Topical Talk**

MM 30.5 Tue 17:00 BAR 205

Soft Matter in Hard Confinement: Molecular Assemblies confined in Nanoporous Solids — ●PATRICK HUBER — Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg

The advent of tailorable nanoporous solids, such as porous silicon and alumina, allows one to explore the equilibrium and non-equilibrium

properties of condensed matter in well-defined, nanostructured geometries. In my talk I will present selected experiments on kinetic and thermodynamic phenomena, ranging from spontaneous imbibition, capillary condensation and glass formation to nematic ordering and crystallization in pores a few nanometers across. Depending on the nature of the basic building block of the molecular assemblies investigated (rare gas molecules, water, liquid crystals, linear hydrocarbons, polymers and proteins) and the mean pore diameter of the porous host a remarkable robustness, however, also substantial deviations from the macroscopic bulk behaviour can be observed, both with regard to the equilibrium and non-equilibrium behaviour.

MM 30.6 Tue 17:30 BAR 205

Polarization discontinuities in two-dimensional honeycomb

lattices — ●MARCO GIBERTINI, GIOVANNI PIZZI, and NICOLA MARZARI — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, Switzerland

The unprecedented and fascinating phenomena taking place at oxide interfaces such as $\text{LaAlO}_3/\text{SrTiO}_3$ have recently triggered the search for their two-dimensional analogues. In this respect, honeycomb lattices seem to offer a rich playground, both for their versatility and the fundamental experimental developments that ensued from the discovery of graphene. In this talk we would like to emphasize, with the help of atomistic first-principles simulations, how to achieve polar discontinuities across interfaces between honeycomb lattices, elucidating the key physical processes that occur and their possible practical applications.

MM 31: Mechanical properties II - Characterisation mechanics

Time: Tuesday 15:45–17:00

Location: IFW D

MM 31.1 Tue 15:45 IFW D

Problems of understanding defect-related mechanical loss spectra in aluminium — ●HANS-RAINER SINNING and JENS BERNHARDT — Institut für Werkstoffe, Technische Universität Braunschweig

Aluminium is one of the most thoroughly studied materials with respect to basic mechanisms of internal friction and anelastic relaxation, such as low-temperature intrinsic dislocation relaxation (Bordoni relaxation), various kinds of dislocation - point defect interactions, grain-boundary sliding, and high-temperature dislocation processes. Although these mechanisms and related phenomena are usually treated separately, they are often overlapping or even physically connected, e.g. by common rate-controlling processes like bulk or short-circuit diffusion. This makes their identification and understanding sometimes difficult, particularly in technical Al-based materials. On the other hand, such understanding is highly desirable because of pronounced effects and high sensitivity of the spectra observed. Here we will discuss some characteristic modifications recently observed mainly in the high-temperature parts of the spectra (around the well-known "grain-boundary peak"), as introduced e.g. by ceramic reinforcements (particles or BN nanotubes), or by severe plastic deformation.

MM 31.2 Tue 16:00 IFW D

Observation of dislocation - related damping mechanisms in Al - based materials — ●JENS BERNHARDT and HANS-RAINER SINNING — Institut für Werkstoffe, Technische Universität Braunschweig, Germany

Damping features in Al based alloys between 100 K and room temperature are due to dislocation dynamics. In metal matrix composites (MMCs) formation of micro plastic deformation zones take place during thermal cycling at the interface between metal matrix and reinforcing phase. As we have shown before a broad damping structure in mechanical loss spectra of annealed AA 6061 based MMC (22 % Al_2O_3) could be assigned to free dislocations generated at the interface between metal matrix and reinforcing particles.

To understand the nature of this broad damping structure we measured damping spectra of Al(99,99), and an Al(99,7) + 10 % B4C composite. In deformed Al(99,99) we observed the Bordoni-Peak around 150 K at 1 kHz. This peak is due to interaction of dislocations with crystal lattice. In Al(99,7) + 10 % B4C a further peak in damping was observed at temperatures between 250 K and room temperature. He is embedded in a broad damping structure comparable to the one observed in AA 6061 + 22 % Al_2O_3 . The mechanism of this peak is most likely dragging of dislocations by point defects (PD) with some enhanced diffusion involved. We will show that this damping peak is depending on heating rate, amplitude of measurement and frequency as well. Properties of Bordoni-Peak, PD-Dislocation Peak and also of the broad damping structure are being discussed for all materials.

MM 31.3 Tue 16:15 IFW D

Ambiguity filtering for quantitative data analysis of ACOM-TEM imaging of nanocrystalline metals — ●AARON KOBLER^{1,2}, EDGAR RAUCH³, CHRISTIAN KÜBEL¹, and HORST HAHN^{1,2} — ¹Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — ²Technische Universität Darmstadt (TUD), Darmstadt, Germany — ³SIMAP laboratory, Saint Martin d'Hères Cedex, France

Automatic Crystal Orientation Mapping for the Transmission Electron Microscope (ACOM-TEM) still is a new technique. It allows investigating nanocrystalline (nc) metals with crystal sizes <100 nm where Electron Backscattering Diffraction reaches its limitations. Recently, we combined ACOM-TEM (Nanomegas) imaging with in-situ straining inside the TEM using Hysitron's TEM Picoindenter to follow up the deformation processes of nc PdAu alloys. After recognizing grains/crystallites in crystal orientation maps using Mtex we tracked individual crystallites through straining series. This allowed us to separate grain rotation from an overall sample bending. However, this tracking fails if the grain recognition is misled by the famous 180° ambiguity of the crystal orientation data. 180° ambiguity arises for certain crystal orientations if the underlying spot diffraction pattern show only a limited number of diffraction spots from the zero order Laue zone. As a result of it twin noise is visible. This kind of noise leads to failure of the crystallite tracking and a reduced reliability of quantitative data analysis. Here we present a simple approach to correct for this ambiguity, further some results on in-situ straining of nc PdAu using this filter.

MM 31.4 Tue 16:30 IFW D

Energetic Structure of micro Laue Peaks from Plastically-Deformed Cu Micro-Beam Revealed by a Three-Dimensional X-ray Detector — ●ALI ABOUD¹, CHRISTOPH KIRCHLECHNER², LOTHAR STRÜDER³, JOZEF KECKES⁴, and ULLRICH PIETSCH¹ — ¹University of Siegen FKP — ²Max Planck Institut für Eisenforschung GmbH — ³PNSensor GmbH — ⁴Material Center Leoben Forschungs GmbH

Energy dispersive micro-Laue diffraction is used to analyse morphology and energetic structure of circular and streaked Cu 711 and 511 reflections collected during a position-resolved experiment on a plastically deformed Cu micro-beam with dimension of $6 \times 6 \times 30 \mu\text{m}^3$. The synchrotron experiment was performed at the BM32 beam line of ESRF using polychromatic radiation of 5-27keV and beam size of $0.5 \times 0.5 \mu\text{m}^2$. The diffraction signal was recorded using an energy-dispersive two dimensional detector; pnCCD. Whereas the Laue reflections obtained from undeformed sample regions remain sharp and diffract at distinct X-ray energies, streaked reflections originating from plastically deformed regions possess an energy gradient which is interpreted by lattice rotation caused by geometrically necessary dislocations stored in the crystal. The novel approach represents a milestone in the structural analysis of materials and will be used to analyse (i) strains in elastically deformed samples without the need of sample rotation and (ii) dislocation structures as well as local strains in plastically deformed metals.

MM 31.5 Tue 16:45 IFW D

The influence of dissolved hydrogen in palladium on the pop-in load — ●MARTIN DEUTGES¹, CHRISTINE BORCHERS¹, and REINER KIRCHHEIM^{1,2} — ¹Institut für Materialphysik, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan

The transition of elastic to plastic deformation in an initial defect free material is accompanied by the creation of a new dislocation loop. Nanoindentation allows to observe this event and the load at which

this happens is called pop-in load.

It is well known that hydrogen affects defect formation. As an example, dissolved hydrogen in palladium facilitates the formation of dislocations, leading to an increase in dislocation density [1].

The palladium-hydrogen system was chosen to analyze this effect with nanoindentation. For this purpose an in-situ setup is used to keep a defined hydrogen concentration within the α -phase of the palladium-

hydrogen system.

These experiments can be analyzed using the defectants concept [2], the basis of which is the assumption that a decrease of the overall free energy by the segregation of solute atoms to a defect can be ascribed to a decrease of the defect formation energy.

[1] Y.Z. Chen et al., *Scripta Mater.* 68 (2013) 743.

[2] R. Kirchheim, *Acta Mater.* 55 (2007) 5129.

MM 32: Transport II - Microstructure/Grain boundaries

Time: Tuesday 15:45–16:45

Location: IFW B

MM 32.1 Tue 15:45 IFW B

Wetting and pre-melting phase transitions in Cu(Bi) alloys studied by tracer diffusion — ●HENNING EDELHOFF¹, BORIS STRAUMAL², SERGIY DIVINSKI¹, and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Institute of Solid State Physics, Chernogolovka, Russia

It is well known that segregation of impurity elements to grain boundaries (GB) can cause a severe change of the material properties. In some systems, e.g. for the Cu-Bi one, the solute (Bi) excess at Cu GBs leads to grain boundary embrittlement (GBE). Due to increasing amounts of GBs in ultrafine grained and nanocrystalline materials and the potential enrichment of Bi in copper-based materials for microelectronic applications, evoked by the usage of Pb-free solders like Sn-Bi or Sn-Ag-Bi in the chip technology, the understanding of the GBE phenomenon in general and in the Cu(Bi) system particularly is of great importance.

Previously, GB diffusion of Cu and Bi in Cu(Bi) alloys has been investigated and kinetic enhancement corresponding to a pre-wetting phase transition was reported [1]. The question arises how the atomic transport of other solutes is influenced by the phenomenon of GBE in the Cu(Bi) system. In this work the GB diffusion of Ag, as one of the main elements in Pb-free solder alloys, in Cu(Bi) alloys is investigated by the radiotracer technique. The effect of segregation, grain size and GB wetting transition on the kinetics of Ag GB diffusion is discussed.

[1] S.V. Divinski, M. Lohmann, Chr. Herzig, B. Straumal, B. Baretzky, W. Gust, *Phys. Rev. B.*, 71, 104 (2005)

MM 32.2 Tue 16:00 IFW B

Transport and structural properties of grain boundaries in ultrafine grained Cu — ●MATTHIAS WEGNER¹, JÖRN LEUTHOLD¹, MARTIN PETERLECHNER¹, DARIA SETMAN², MICHAEL ZEHETBAUER², SERGIY V. DIVINSKI¹, and GERHARD WILDE¹ — ¹Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Straße 10, D-41849, Germany — ²Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria

According to existing models of grain refinement by severe plastic deformation, the abundance of lattice dislocations created during the severe straining serves to modify the grain boundary structure of general high angle grain boundaries (GHAGB) towards a state with an enhanced excess free energy density. The hereby modified microstructure of 4N Cu, processed by High Pressure Torsion (HPT), tends to recrystallize already at low homologous temperatures of about 0.26 revealing a significant decrease in the recrystallization temperature. Diffusion in these structures features "ultra fast" in addition to "conventional" rates of grain boundary diffusion along GHAGB (as present in annealed coarse-grained polycrystals). The results indicate a special microstructural state of at least a fraction of interfaces (suitable for percolation) which relax, but are still observable at 320 K. Diffusion experiments above 320 K involve a complete recrystallization of the initial structure. Fast diffusion rates are still measurable featuring the presence of "High Energy Grain Boundaries" (HEGB) in recrystallized HPT Cu.

At temperatures higher than 443 K, microstructural relaxation induces a further transformation of HEGB into GHAGB.

MM 32.3 Tue 16:15 IFW B

Diffusion and microstructure in ultrafine grained nickel — ●SIMON TRUBEL, SERGIY DIVINSKI, MARTIN PETERLECHNER, GERHARD WILDE — Institut für Materialphysik der Westfälischen Wilhelms-Universität

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 show ultra-fast diffusion rates in severely deformed materials created by equal channel angular pressing (ECAP) [1]. Further investigations on pre-annealed ECAP-Nickel were conducted to analyse the nature of its recovery on a microscopic scale. In order to analyse the impact of the strain path and particularly of the hydrostatic component of the applied stress, the material of the same starting ingot has also been applied to high pressure torsion (5 turns, 2 GPa applied pressure). Grain boundary self-diffusion has been analysed by applying 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 and characteristics by SPD.

MM 32.4 Tue 16:30 IFW B

Lattice degradation in bi-crystalline Ag wires during reversible electromigration — ●SIMON P. SINDERMANN, MICHAEL HORN-VON HOEGEN, GÜNTER DUMPICH, and FRANK-J. MEYER ZU HERINGDORF — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE) University of Duisburg-Essen, D-47057 Duisburg, Germany

Electromigration is known as the reversible mass transport occurring at high electric current densities. We use well controlled bi-crystalline Ag test structures [1] to study the interaction of electromigration driven voids with the crystal lattice by *in-situ* scanning electron microscopy (SEM).

Previously we have shown that the void shape is strongly influenced by the lattice symmetry [2], and we observed an increased number of additional voids in the motion path of voids [3].

Here, we present our observation of void motion at the reversal of the electric current direction. We find that a void exactly retraces its previous path. The test structure remembers where a void has passed through it. Electron backscatter diffraction (EBSD) shows that this kind of memory effect is caused by a permanent lattice degradation. Electromigration is thus not reversible with respect to the microstructure.

[1] S. Sindermann et al. *RSI* **82**, 123907 (2011)

[2] A. Latz et al. *PRB* **85**, 035449 (2012)

[3] S. P. Sindermann et al. *JAP* **113**, 134505 (2013)

MM 33: Nanomaterials II - Tubular nanostructures

Time: Tuesday 15:45–17:45

Location: IFW A

MM 33.1 Tue 15:45 IFW A

Synthesis, characterization and electrical properties of copper coated multi-walled carbon nanotubes — ●ABDELWAHAB HASSAN, SILKE HAMPEL, ESLAM IBRAHIM, CHRISTIAN HESS, ALBRECHT LEONHARDT, and BERND BÜCHNER — Leibniz-Institute for Solid State and Materials Research (IFW-Dresden), D-01171 Dresden, Germany

In the recent years, carbon nanotubes (CNTs) have received considerable attention as new materials for a variety of potential applications due to their interesting properties. As well as, CNT- can be reinforced metal matrix composites (MMCs). The coating of CNTs with metal and metal oxide is fundamentally important for applications of CNTs in nanoelectronic device, gas sensor and composite materials, etc. As well as coating of CNTs lead to a significant improvement of interfacial bond between CNTs and metal matrix. Therefore, in the present contribution, a novel route to synthesize copper/multi-walled carbon nanotubes (MWCNTs) was developed using a chemical electroless plating process after the radio frequency (RF) plasma treatment of the CNTs. Plasma treatment of MWCNTs surface was carried out in various gaseous atmospheres, namely Ar, H₂ and N₂ to improve copper adhesion. N₂ plasma treatment showed better surface activation of the MWCNTs. This study investigated the effect of plasma treatment time, flow rate and RF power to improve the copper coating. The morphology of MWCNTs were studied by TEM, SEM, Raman spectroscopy, XPS as well as X-ray diffraction (XRD). The measurements of electrical conductivity of uncoated and copper coated MWCNTs were measured by four-point method in temperature range 300-573 K.

MM 33.2 Tue 16:00 IFW A

Growth of periodic arrays of perpendicularly aligned multi-walled carbon nanotubes — ●ESER METIN AKINOGLU, ANTHONY JOHN MORFA, and MICHAEL GIERSIG — Freie Universität Berlin, Department of Physics, Berlin, Germany

Multi-walled carbon nanotubes (MWCNTs) are promising nano materials with unique properties such as their extraordinary mechanical strength and their electrical conductivity. Using a combination of nanosphere lithography (NSL) for catalyst nano-patterning and plasma enhanced chemical vapor deposition (PECVD) for perpendicularly aligned growth we can produce different MWCNT systems. NSL utilizes a hexagonally close packed monolayer of submicron polystyrene spheres (PSS) as a lithography mask for metal deposition. A periodic array of triangular shaped metal islands remains after chemically removing the PSSs. The size and distance in between the metal islands can be tuned by enlarging or shrinking the hexagonal unit cell which can be tuned through the used PSS size. In the PECVD of MWCNTs a vapor-liquid-solid growth process is used where nickel acts as a catalyst and as a protective helmet during ion bombardment for perpendicular MWCNT growth. By changing the catalyst pretreatment, plasma conditions, growth temperature, gas composition and growth time of the PECVD process we can vary the MWCNT growth kinetics yielding vastly different results in terms of shape, size and crystallinity. In this presentation we show the optimization of parameters for MWCNT growth and discuss potential bio and energy applications such as antimicrobial surfaces and field emitter arrays.

MM 33.3 Tue 16:15 IFW A

Investigation of the antimicrobial activity of well-dispersed multiwalled carbon nanotubes (MWCNT) — ●MARYAM KHAZAEI¹, DAN YE¹, ANINDYA MAJUMDER¹, LARYSA BARABAN¹, JÖRG OPITZ^{1,2}, and GIANAURELIO CUNIBERTI^{1,3} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ²Fraunhofer Institute IZFP Dresden, 01109 Dresden, Germany — ³Division of IT Convergence Engineering, POSTECH, Pohang, Korea

Antimicrobial activity of well-dispersed MWCNTs with an average diameter of 10 nm was investigated by analyzing the growth curves of Escherichia coli (E.coli) population in surfactant-modified MWCNTs and polymer-modified MWCNTs in Luria Bertani (LB) broth. MWCNTs can be dispersed in ionic surfactants like sodium dodecyl sulfate (SDS), sodium dodecylbenzenesulfonate (SDDBS), sodium cholate (SC), dodecyltrimethylammonium bromide (DTAB) and decyltrimethylammonium bromide (CTAB), as well as in a non-ionic polymer-polyvinylpyrrolidone (PVP). Good dispersion of surface func-

tionized MWCNTs was observed by UV-Vis spectroscopy and microscopic techniques. Biocompatibility of these surfactants was estimated by analyzing the growth curves of E. coli population in both surfactant-LB broth and polymer-LB broth. SDDBS and PVP, which showed the least toxicity towards the E. coli cells, were selected to study the interaction of well-dispersed MWCNTs by these materials with bacteria. Observation of the deformed E.coli cell membranes using SEM confirms the antimicrobial activity of MWCNTs.

MM 33.4 Tue 16:30 IFW A

Investigation of the antimicrobial activity of well-dispersed multiwalled carbon nanotubes (MWCNT) — ●MARYAM KHAZAEI¹, DAN YE¹, ANINDYA MAJUMDER¹, LARYSA BARABAN¹, JÖRG OPITZ^{1,2}, and GIANAURELIO CUNIBERTI^{1,3} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ²Fraunhofer Institute IZFP Dresden, 01109 Dresden, Germany — ³Division of IT Convergence Engineering, POSTECH, Pohang, Korea

Comparative dispersion capability of ionic surfactants like Sodium dodecyl sulfate (SDS), Sodium dodecylbenzenesulfonate (SDDBS), Sodium cholate (SC), Dodecyltrimethylammonium bromide (DTAB) and Decyltrimethylammonium bromide (CTAB) and a non-ionic polymer- Polyvinylpyrrolidone (PVP) was examined to disperse MWCNTs. The surface functionalized dispersed MWCNTs with average diameter of 10 nm were investigated using microscopic techniques. Among these surfactants, SDDBS and DTAB provided maximum and minimum dispersion susceptibility, respectively. Furthermore, different concentrations of PVP showed good capabilities for MWCNTs dispersion. Biocompatibility of these surfactants and polymer was estimated by analyzing their optical density (OD) growth curves after treating them with E.coli. SDDBS and PVP which showed the least toxicity, were selected to study their biocompatible interaction with well dispersed MWCNTs. Observation of the deformed E.coli cell membranes confirm the antimicrobial activity of MWCNTs.

15 min break

MM 33.5 Tue 17:00 IFW A

Unveiling the atomic structure of single-wall boron nanotubes — ●JENS KUNSTMANN^{1,2}, VIKTOR BEZUGLY^{2,3}, HAUKE RABEL², and GIANAURELIO CUNIBERTI^{2,3} — ¹Department of Chemistry, Columbia University, 3000 Broadway New York, NY 10027, USA — ²Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ³Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

Despite recent successes in the synthesis of boron nanotubes (BNTs), the atomic arrangement of their walls has not yet been determined and many questions about their basic properties do remain. Here, we unveil the dynamical stability of BNTs by means of first-principles molecular dynamics simulations. We find that free-standing, single-wall BNTs with diameters larger than 0.6 nm are thermally stable at the experimentally reported synthesis temperature of 870 degrees Celsius and higher. The walls of thermally stable BNTs are found to have mixed triangular-hexagonal morphologies. The latter could develop into a new structural paradigm in boron chemistry.

MM 33.6 Tue 17:15 IFW A

From metal to semiconductor: an *ab initio* study of chemically functionalized boron nanotubes — ●VIKTOR BEZUGLY^{1,2}, HERMUT MICHAEL ZOPF¹, JENS KUNSTMANN^{1,3}, and GIANAURELIO CUNIBERTI^{1,2,4} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — ²Center for Advancing Electronics Dresden, TU Dresden — ³Department of Chemistry, Columbia University, 3000 Broadway, New York — ⁴Dresden Center for Computational Materials Science, TU Dresden

Nanotubes of elemental boron have been synthesized in recent years [1]. In contrast to carbon nanotubes (CNTs), boron nanotubes (BNTs) are metallic independent of their diameter and chirality and have higher conductivity than metallic CNTs [1,2]. In our DFT investigations we show how chemical functionalization of single-walled BNTs can tune the basic electronic properties from metallic to semiconducting. The effect can be achieved by atoms or functional groups which have a par-

ticular chemical bonding interactions with BNTs. Our result indicate that functionalization of BNTs offers chirality independent control of the electronic structure of the nanotubes, which is paramount for industrial applications.

[1] F. Liu *et al.*, *J. Mater. Chem.* **20**, 2197 (2010); J. Liu, Z. Iqbal, *MRS Online Proc. Lib.* **1307** (2011) DOI: 10.1557/opl.2011.320.

[2] V. Bezugly *et al.*, *ACS Nano* **5**, 4997 (2011).

MM 33.7 Tue 17:30 IFW A

Electronic structure calculations of modified diamondoids — ●BIBEK ADHIKARI and MARIA FYTA — Institute for Computational Physics, Stuttgart, Germany

Diamondoids are diamond like cage structure with hydrogen terminations, which have tremendous potential for nanotechnological applica-

tions. We focus on alteration and structural modifications of diamondoids by doping these molecules with various elements. We perform density functional theory based calculations to reveal the electronic properties of these doped diamondoids. We plan to investigate the position of the dopants with respect to the cage structure for lower as well as higher diamondoids and reveal the stability and structural characteristics with respect to different doping sites. We next turn to the study of selective functionalization of these molecules. We functionalize two sites of the same diamondoid with a thiol and amine group, respectively. In the end, we discuss the effect of functionalization of self-assembled diamondoid monolayers. The aim is to selectively tune the optical and electronic properties of diamondoids with dopants and/or functionalization groups in view of their novel nanotechnological applications.

MM 34: Poster Session

Time: Tuesday 18:00–20:00

Location: P4

MM 34.1 Tue 18:00 P4

Simulation of abnormal grain growth in nanocrystalline materials — ●MINGYAN WANG¹, JULES DAKE¹, RAINER BIRRINGER², and CARL KRILL¹ — ¹Institute of Micro and Nanomaterials, Ulm University, Germany — ²FR 7.3 Technical Physics, University of the Saarland, Germany

Despite the rarity suggested by its name, abnormal grain growth (AGG) appears to be a common mode of coarsening in nanocrystalline specimens, observed in a wide variety of materials prepared by a range of synthesis routes. During AGG, a subpopulation of grains manifests rapid growth, leading to grain volumes that are not only much larger than those of their neighbors, but also sometimes highly irregular in shape. The latter observation suggests that, in certain cases, AGG might proceed by a kind of percolation phenomenon occurring on a “grid” defined by the initial ensemble of grains. We have investigated this possibility by extending a conventional phase field algorithm for simulating grain growth to include selection rules for percolation. The resulting simulated abnormal grains are strikingly similar in shape to their experimental counterparts. By quantifying the comparison between simulation and experiment, we hope to shed light on at least one of the underlying physical mechanisms for AGG in nanocrystalline materials.

MM 34.2 Tue 18:00 P4

Grain boundary enthalpy changes by mechanical deformation of nanocrystalline alloys — ●MICHAEL DECKARM¹, JONATHAN SCHÄFER², PATRIC GRUBER³, KARSTEN ALBE², and RAINER BIRRINGER¹ — ¹Universität des Saarlandes, FR 7.2 Experimentalphysik, 66123 Saarbrücken — ²Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, 64281 Darmstadt — ³Karlsruher Institut für Technologie, Institut für Angewandte Materialien, 76344 Eggenstein-Leopoldshafen

In as-prepared nanocrystalline (nc) alloys, grain boundaries (gb) are usually in unknown local non-equilibrium configurations, reflecting the preparation history. However, a thermally activated recovery process below the onset temperature of grain growth permits a local equilibration of the gb and thus providing a well defined reference state.

Starting from this reference state we deformed nc (alloy) samples by uni-axial compression and investigated the change of gb enthalpy as a function of plastic strain by calorimetry. The experimental findings are in large parts in excellent agreement with the results of a hybrid MD/MC simulation method for the same material.

Surprisingly, annealing leads to significantly increased yield stresses and narrowing of the microplastic regime in uniaxial compression tests. Obviously, the configurational state of the gb seems to significantly influence the overall mechanical behaviour of nc metals at the low end of the nanoscale.

MM 34.3 Tue 18:00 P4

Optimization of a Nanocalorimeter inside an SEM — ●EMANUEL FRANKE¹, CYNTHIA A. VOLKERT¹, FENG YI², and DAVID A. LAVAN² — ¹Institut für Materialphysik, Georg-August-University, Göttingen, 37077 Göttingen — ²Materials Measurement Science Division, Material Measurement Laboratory, National Institute of Stan-

dards and Technology, Gaithersburg, USA 20899

As sample length scales reach down to nanometers and the surface to volume ratio becomes large, the thermal properties of materials are changed. The involved energy in such size induced changes is often only a few nano-Joules and cannot be measured by conventional calorimetry which has too low sensitivity. MEMS-based nanocalorimeters with sufficient resolution to measure with nJ resolution have been developed in the last two decades. We present several proof-of-concept experiments using a MEMS based differential calorimeter which has been installed in a field emission SEM. The SEM allows careful observation of the experimental conditions and of any changes in the sample microstructure due to thermal cycling. Enthalpy change can be measured from room temperature up to 1000 K by applying heating rates from 10⁴ K/s to 10⁵ K/s. Sensitivity better than 1 nJ/K for reversible and 10 nJ/K for irreversible processes can be achieved. The limits of the measurement method are explored by studying dewetting and oxidation of copper films and melting of bismuth nanoparticles.

MM 34.4 Tue 18:00 P4

Spatial and orientational tracking of Ostwald ripening in semisolid Al-Cu by 3DXRD microscopy — ●JAMES C. SHATTO¹, JULES DAKE¹, THOMAS WERZ¹, JETTE ODDERSHEDE², HENNING SØRENSEN³, SØREN SCHMIDT², and CARL KRILL¹ — ¹Inst. of Micro and Nanomaterials, Ulm University, Germany — ²Dept. of Physics, Technical University of Denmark — ³Dept. of Chemistry, University of Copenhagen, Denmark

Coarsening, a phenomenon that occurs whenever a polycrystalline material is subjected to thermal processing, has long been a favorite topic of materials scientists. Examples include grain growth (in single-phase samples) and Ostwald ripening (in multiphase materials). Using the relatively new technique of Three-Dimensional X-Ray Diffraction (3DXRD) microscopy, we have investigated the coarsening-induced growth/shrinkage of solid, Al-rich particles embedded in a liquid matrix (of higher Cu content). The measurement technique reveals not only the spatial extent of each crystalline particle but also its lattice orientation at discrete time steps. From this information we can study the migration rates of individual particle boundaries as a function of relative lattice misorientation across the boundary. Such data may yield the first experimental differentiation between the conventional mechanism for Ostwald ripening (atomic diffusion through the second phase) and particle growth via coalescence or diffusion of atoms across single-phase interfaces.

MM 34.5 Tue 18:00 P4

Cooling rate dependend short and medium range order of a CuZrAl glass analyzed by comparing XRD data and MD simulations — ●HELMUT HERMANN¹, VALENTIN KOKOTIN², UTA KÜHN¹, BJÖRN SCHWARZ³, IVAN KABAN⁴, and HORST WENDROCK¹ — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden — ²ThyssenKrupp Steel Europe AG, Kaiser-Wilhelm-Str. 100, 47166 Duisburg — ³Karlsruhe Inst. of Technology, IAM-ESS, Hermann-von Helmholtz-Platz 1, 76344 Eggeningen-Leopoldshafen — ⁴TU Dresden, Inst. für Werkstoffwissenschaft, 01062 Dresden

The preparation of a CuZrAl glass is simulated at different cooling rates by means of molecular dynamics (MD). The atomic order is

studied using generalized Voronoi tessellation. It appears that the fraction of icosahedral Voronoi cells increases with decreasing cooling rate. These differences are visible in changes of the X-ray scattering intensities of the simulated samples. Parallel to the simulations, samples with the same composition are prepared experimentally under different cooling rates which are realized by means of rapid quenching and mould casting techniques, respectively. Synchrotron radiation is used to measure the diffraction curves of the samples. The experimental X-ray scattering curves for the samples obtained at different cooling rates show the same features as the curves calculated from the samples generated by MD simulation at different cooling rates. This confirms the simulation results.

MM 34.6 Tue 18:00 P4

Visualization of scattering properties by Neutron Grating Interferometry — ●BENEDIKT BETZ¹, EBERHARD LEHMAN¹, RUDOLF SCHAEFER^{2,3}, PETER RAUSCHER³, and CHRISTIAN GRUENZWEIG¹ — ¹SINQ, Paul Scherrer Institut, Villigen, Switzerland — ²IFW, Dresden, Germany — ³Technische Universität Dresden, Dresden, Germany

The neutron Grating Interferometer (nGI) is a standard user instrument at the ICON beamline at SINQ at PSI. The setup is able to deliver simultaneously information about the attenuation, phase shift [1] and scattering properties in the so called dark-field image (DFI) [2] of a sample. Due to the interaction of neutrons with the nucleus only, they are able to penetrate deeper into matter, in particular heavier materials, than X-rays do. A further advantage of neutrons compared to X-rays is the interaction of the neutrons* magnetic moment with magnetic structures, that allows for the investigation of magnetic domain structures using the nGI technique [3]. In the forseen talk, the nGI-setup and its technique for imaging with cold neutrons will be explained. In the forseen talk, the nGI-setup and its technique for imaging with cold neutrons will be explained. Furthermore examples for the investigation of magnetic structures in Grain-oriented and non-oriented steel laminations (FeSi) will be presented. [1]:F. Pfeiffer et al. Neutron phase imaging and tomography, Phys. Rev. Lett. 96, 215505, (2006)[2]:C.Grünzweig et al. Neutron Decoherence Imaging for Visualizing Bulk Magnetic Domain Structures. Phys. Rev. Lett. 101, 025504 (2008) [3]:C.Grünzweig et al. Bulk magnetic domain structures visualized by neutron dark-field imaging. Appl. Phys. Lett. 93, 112504(2008)

MM 34.7 Tue 18:00 P4

Influence of different loading stresses to duplex steel in the VHCF regime — ●ANNE HÜSECKEN¹, MARCUS SÖKER², KONSTANTIN ISTOMIN¹, BENJAMIN DÖNGES¹, and ULLRICH PIETSCH¹ — ¹Universität Siegen — ²Hochschule Osnabrück

Damage mechanisms in the VHCF regime are still not sufficiently understood. Experiments on austenitic-ferritic duplex steels up to 10⁹ cycles have revealed that elastic anisotropy causes stress concentrations at grain and phase boundaries leading to slip band emanation preferentially in the fcc austenite phase [1]. Slip bands raise locally the residual stress level in the neighbouring bcc ferrite grains. So, crack initiation along pronounced slip bands and grain/phase boundaries were observed [1,2]. There is a need to analyse the development of dislocations and their formation to slip bands within the grains in order to correlate the observed microstructure with relevant damage mechanisms. We present a new way of fatigue analysis measuring the change of shape of selected austenite and ferrite X-ray Bragg reflections for single grains as function of the number of VHCF cycles and different loading stresses in-situ. It was explored that selected austenite reflections show an increasing peak splitting as function of load cycles whereas ferrite reflection kept nearly unchanged. This finding can be attributed to the formation of stress induced dislocations bunches in austenite grains which may acts as nuclei for crack formation in neighbouring ferrite grains [3]. [1] U. Krupp: Fatigue Crack Propagation in Metals and Alloys (Wiley, 2007). [2] H. Knobbe et al, J. Phys.: Conf. Ser. 240 (2010) 012061 [3] K.Istomin et .al. Fatigue, submitted 2013

MM 34.8 Tue 18:00 P4

Simulation of Grazing-Incidence Small-Angle Scattering on Cu nano-size clusters — CELINE DURNIK¹, ●MARINA GANEVA¹, CHRISTIANE A. HELM², RAINER HIPPLER², OXANA IVANOVA¹, GENNADY POSPELOV¹, WALTER VAN HERCK¹, and JOACHIM WUTTKE¹ — ¹Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — ²Institut für Physik, Universität Greifswald, Greifswald, Germany

Grazing-incidence small-angle scattering (GISAS) is increasingly used

to investigate the structural properties of thin films, layered materials, deposited nanoparticles and many others. To prepare a successful experiment and to analyze the measured data, appropriate simulations are required.

BornAgain [1] is a multi-platform open-source project that aims at supporting scientists in the analysis and fitting of their GISAS data, both for synchrotron (GISAXS) and neutron (GISANS) facilities. It is provided with a sample model and an instrument model accounting for the resolution effects, and simulates the scattering process using the distorted-wave Born approximation (DWBA).

Here we show GISAXS and GISANS images simulated using BornAgain. The influence of the sample properties and experimental parameters on the scattering pattern is discussed. Cu clusters, produced using a DC magnetron-based gas aggregation source and deposited to a Si substrate, are taken as a case study.

[1] <http://apps.jcnsc.fz-juelich.de/doku/sc/bornagain:start>

MM 34.9 Tue 18:00 P4

Heterogeneous shear elasticity of glasses: Instability, anharmonicity and fractional-power scaling — ●WALTER SCHIRMACHER^{1,2}, ALESSIA MARRUZZO^{2,3}, ANDREA FRATALOCCHI³, GIANCARLO RUOCCO², and TULLIO SCOPIGNO² — ¹Institut für Physik, Universität Mainz, Germany — ²Dipt. of Fisica, Universit'a "La Sapienza", Italy — ³Faculty of Electr. Eng., Applied Mathematics and Computational Science, King Abdullah University of Science and Technology, Saudi Arabia

Dynamical heterogeneity is the hallmark of glassy dynamics both on the liquid and on the solid side of the glass transition. On the solid side elastic heterogeneity causes a wealth of anomalous vibrational phenomena such as an enhancement of the vibrational spectrum over the Debye expectation ("boson peak") and anomalous sound dispersion and attenuation. Above the boson peak frequency region the anomalies are entirely due to harmonic degrees of freedom and are caused by the disorder-induced breakdown of translational invariance. Below this region - as we report here by comparing experimental sound attenuation data with simulations on a soft-sphere glass and an appropriate theory - there develops a dynamical scaling scenario caused by the combined action of disorder, local instability and anharmonicity.

MM 34.10 Tue 18:00 P4

Showdown! Comparing phase field simulations to time-resolved x-ray tomography measurements of Ostwald ripening in 3D — THOMAS WERZ¹, NAN WANG², MICHAEL HEINZE³, STEFAN ODENBACH³, LONG-QING CHEN², and ●CARL KRILL¹ — ¹Inst. of Micro and Nanomaterials, Ulm University, Germany — ²Dept. of Materials Science and Engineering, The Pennsylvania State University, USA — ³Inst. of Fluid Mechanics, TU Dresden, Germany

It's not only moviegoers whose imagination has been captured by the 3D revolution in imaging technology—even materials scientists have been swept up in the hype. Their excitement is understandable, given the power of techniques like x-ray microtomography to map out microstructural evolution with high spatial and temporal resolution. However, not everyone believes that the resulting 3D "movies" are worthy of Oscar consideration: after all, computational materials scientists have generated thousands of 3D simulations without winning a single Academy Award! Perhaps voters are still waiting for the computational algorithms to be validated against experiment. We have addressed the latter issue by investigating Ostwald ripening in the model system Al-5 wt% Cu, using x-ray microtomography to obtain real-time 3D image sequences of particle growth and shrinkage. We then employed a phase-field model to simulate coarsening in the same sample region, starting from the measured initial configuration. The stage is now set for a showdown in 4D (3 spatial dimensions + time) between experiment and computer simulation. The results could decide once and for all whether theorists can lay claim to simulating reality!

MM 34.11 Tue 18:00 P4

The Grain Mapper at the High Energy Beamline HEMS — ●TORBEN FISCHER, LARS LOTTERMOSER, SVEN KLEEBAND, NORBERT SCHELL, MARTIN MÜLLER, and ANDREAS SCHREYER — Helmholtz-Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht, Germany

The 3D investigation of polycrystalline materials allows the study of the relationship between macroscopic and micro structural properties at the level of single grains. A main objective is the measurement of the 3D strain state between single grains. The High Energy Materials Science Beamline (HEMS), operated by the Helmholtz-Zentrum

Geesthacht (HZG), has a dedicated hutch for such 3D techniques. HEMS is situated at the high brilliance synchrotron storage ring PETRA III at DESY in Hamburg and has a tuneable energy range between 30 and 200 keV. Fast detector systems and high photon flux allow for highly dynamic investigations, e.g. of phase transformation or catalysis. The X-ray beam can be focused down to micrometre size with compound refractive lenses (CRLs). The grain mapper is an optimized endstation for the 3D-XRD technique. The grain mapper consists of a solid granite substructure, a high precision rotation stage and portals for far- and near-field detectors. The instrument has finished commissioning phase and first results will be presented. The main scientific topics addressed are the investigation of new joining and machining processes, metallurgy, chemistry and material physics.

MM 34.12 Tue 18:00 P4

Ordered Mesoporous Thin Films; Elastic Modulus Determination by Humidity Driven Pore Lattice Deformation — ●PARVIN SHARIFI¹, BENEDETTA MARMIROLI², BARBARA SARTORI², FERNANDO CACHO-NERIN^{2,3}, HIENZ AMENITSCH², CHRISTIAN GANSER¹, CHRISTIAN TEICHERT¹, and OSKAR PARIS¹ — ¹Institut für Physik, Montanuniversität Leoben (Franz-Josef Strasse 18, 8700 Leoben, Austria) — ²Institute of Inorganic Chemistry, TU Graz (Stremayrgasse 9/IV, 8042 Graz, Austria) — ³Current address: Beamline I14, Diamond Light Source, Harwell Science and Innovation Campus, OX11 0DE Didcot (Oxfordshire), UK

Adsorption induced deformation of mesoporous powders and thin films can provide valuable information about their mechanical properties. Two types of mesoporous thin films were prepared by dip- and spin-coating on silicon substrates using a sol made of TEOS and triblock copolymer (P123) in acidic solution followed by calcination at 400°C. GISAXS measurements revealed ordered mesoporous films with 2D hexagonal structure with a macroscopic alignment of the pore axis within the plane of the substrate. The pore-lattice deformation due to adsorption of water was determined by in-situ GISAXS in a relative humidity range of RH=5% to RH=95%. Both films showed a reversible out-of-plane contraction due to the condensation of water in the pores. Pore lattice strain vs RH, called strain isotherms, were used to determine the *pore load modulus* of the films. The results showed clear differences between the two types of samples.

MM 34.13 Tue 18:00 P4

In-situ tomography on the magnetostructural transition of La(Fe,Si)13 — ●ANJA WASKE¹, BRUNO WEISE^{1,6}, KONSTANTIN SKOKOV², STEFAN SCHMIEDERER^{3,4}, ALEXANDER RACK³, WOLFGANG LUDWIG⁵, OLIVER GUTFLEISCH², and JÜRGEN ECKERT^{1,6} — ¹IFW Dresden, Institute for Complex Materials, Dresden, Germany, — ²TU Darmstadt, Department of Materials Science, Darmstadt, Germany, — ³European Synchrotron Radiation Facility, Grenoble, France, — ⁴University of Manchester, X-ray Imaging Facility, School of Materials, UK, — ⁵GEMPPM-MATEIS, INSA de Lyon, Lyon, France, — ⁶Institute of Materials Science, Dresden University of Technology, 01062 Dresden, Germany

Magnetocaloric material of the composition La(Fe,Si)13 shows a magnetostructural transition connected to a volume expansion of up to 1.5%, which can be induced either by applying a magnetic field or by lowering the temperature below the material's Curie temperature. We conducted a temperature dependent study of this magnetostructural transition to study how the nucleation of the low-temperature state proceeds in the sample as the temperature is lowered. Powderized and bulk samples were compared to study the influence of the neighbouring particles and the constraints those present for other particles (or grains) to transform.

MM 34.14 Tue 18:00 P4

Combined X-ray/Neutron reflectometer NREX - advanced tool for studying surfaces films and heterostructures — ●OLAF SOLTWEDEL, YURY KHAYDUKOV, THOMAS KELLER, FRANZ TRALMER, MANFRED OHL, and BERNHARD KEIMER — MPI für Festkörperforschung, Heisenbergstraße 1, 70569, Stuttgart

This presentation will introduce neutron reflectometry, a unique tool to investigate properties of thin films like chemical composition, interdiffusion, magnetic depth profiling etc. in buried films and dedicated sample environments on nanometre scale. Besides few theoretical aspects scientific applications ranging from polymer films at the solid/liquid interfaces over chemical depth profiling in amorphous hydrogenated carbon to magnetic thin films are presented. Finally, the realisation of a combined x-ray and neutron reflectometer will be

shown in details. Here at the NREX reflectometer (FRM2, Garching, Germany) a conventional X-ray (Cu-K α : $\lambda = 1.541\text{\AA}$) add on offers the unique possibility to combine X-ray and neutron reflectometry in-situ.

MM 34.15 Tue 18:00 P4

In-situ high energy x-ray diffraction studies on the phase evolution during decomposition of arc evaporated (Ti,-Cr,-Al)N coatings — ●DANIEL M. OSTACH¹, NORBERT SCHELL¹, ANDREAS SCHREYER¹, JENS BIRCH², JEREMY SCHROEDER², LINA ROGSTRÖM³, MATTS P. JOHANSSON-JÖEASAAR⁴, and RACHID M'SAOUBI⁴ — ¹Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Max-Planck-Straße 1, 21502 Geesthacht — ²Thin film physics, IFM, Linköping University, 581 83 Linköping, Sweden — ³Nanostructured materials, IFM, Linköping University, 581 83 Linköping, Sweden — ⁴SECO Tools AB, Fagersta, Sweden

Hard and wear resistant cubic (c)-(Ti,Al)N based coatings are widely used in industrial applications, as in the case of coated metal cutting tools. During cutting, the coated tool is exposed to high temperatures and large forces. c-(Ti,Al)N decompose in two stages under such conditions; first a spinodal decomposition into coherent c-TiN and c-AlN rich domains followed by a second stage where c-AlN transforms to hexagonal (h)-AlN. Alloying of Cr in (Ti,Al)N coatings provide an additional decomposition route through the formation of intermediate c-(Al,Cr)N and c-(Ti,Cr)N ternary phases prior to the final stage when h-AlN and c-(Ti,Cr)N are formed. In effect, Cr in (Ti,Al)N has shown to delay the detrimental effect of h-AlN on the coating's hardness. In this study, in-situ high-energy synchrotron x-ray diffraction studies during annealing have been performed to study the phase evolution during decomposition of (Ti,Al,Cr)N coatings.

MM 34.16 Tue 18:00 P4

Development and integration of an intelligent detector for grating based phase-contrast tomography — ●PAVEL LYTAEV¹, FELIX BECKMANN¹, JULIA HERZEN¹, ALEXANDER HIPPI¹, STEPHAN MEYER-LOGES¹, JOERN PLEWKA¹, ANDREAS KOPMANN², MICHELE CASELLE², and ANDREAS SCHREYER¹ — ¹Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Karlsruhe Institute of Technology, Karlsruhe, Germany

Helmholtz-Zentrum Geesthacht (HZG) is operating the microtomography stations using synchrotron radiation at DESY, Hamburg. Absorption contrast and phase contrast techniques were developed and applied to samples in the fields of medicine, biology, and materials science. The present work is devoted to the development of an intelligent detector with high-speed data capturing for experiments for grating based phase-contrast imaging. The detector is based on the Ultrafast streaming camera platform developed at the Karlsruhe Institute of Technology (KIT). Characterization (in terms of photon transfer curve) of some different cameras, such as CMOS and CCD, is presented. These characteristics are required to optimize the operation of the detector according to the one or to the other requirements of processing speed and image quality in the course of phase-contrast imaging process. The detector will be optimized to its implementation at the microtomography setups installed at the beamlines IBL and HEMS of the high brilliant third-generation synchrotron light source PETRA III.

MM 34.17 Tue 18:00 P4

Band gap measurement of SiC nanowires by Valence EELS — ●ANJA BONATTO MINELLA^{1,2}, DARIUS POHL¹, CHRISTINE TÄSCHNER¹, ROLF ERNI³, LUDWIG SCHULTZ^{1,2}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Dresden, Germany — ²TU Dresden, Dresden, Germany — ³Electron Microscopy Center, Empa, Dübendorf, Switzerland

Silicon carbide (SiC) nanowires (NW) of different polytypes have been prepared by Plasma-Enhanced Chemical Vapour Deposition. Their formation proceeds simultaneously with the growth of carbon nanofibres (CNF) leading to a heterostructure of SiC-filled CNF. In order to study the band gap of the SiC the graphitic layers of the CNF have to be removed by a heat treatment in oxygen atmosphere.

The (direct) band gap measurement is carried out using Valence Electron Energy Loss Spectroscopy (VEELS). SiC NW are found to exhibit a large direct band gap of 5.5 eV irrespectively of their polytype. Simulations using the optical properties of cubic SiC and DFT calculations show a similarly large value.

Another feature of the deconvoluted spectrum (after the removal of the zero loss peak) is the occurrence of energy losses that precede the onset of the band gap. This is probably caused by retardation losses or surface states. Possible ways of describing these residual features

will be discussed, and the value of the band gap will be compared to reference data.

MM 34.18 Tue 18:00 P4

one-dimensional metal nanowire arrays prepared by hard-template synthetic method for SERS — ●YONG-TAE KIM¹, STEFAN L. SCHWEIZER¹, and RALF B. WEHRSPHON^{1,2} — ¹Martin-Luther-University Halle-Wittenberg, Halle, Germany — ²Fraunhofer Institute for Mechanics of Materials, Halle, Germany

One-dimensional nanostructures such as nanowire and nanotube arrays have been intensively investigated due to its novel magnetic and optical properties depending on dimensional and size reduction. Especially in case of one-dimensional nanowire arrays with periodic structure, their applications will be extended to many devices for example biosensors, photonic crystals, and electro chemical devices. Therefore the fabrication of one-dimensional nanowire arrays with controlled morphologies and compositions becomes more important on a large scale.

Metal nanowire arrays with high aspect ratio have been prepared using a number of techniques including electron beam or focused ion beam (FIB) lithography, vapor-solid-liquid (VLS) growth process, and template synthetic method. Among these methods, template synthetic method is one of most promising one as increasing emphasis is placed on low cost, high throughput, and ease of production.

In this study, one-dimensional metal nanowire arrays composed of nickel, silver, and gold with single- or multi-segmented structures have been fabricated by electrochemical deposition method using AAO hard template. And these one-dimensional metal nanowire arrays will be estimated as highly active surface-enhanced Raman scattering (SERS) substrates.

MM 34.19 Tue 18:00 P4

Impact of hydrodynamic parameters on the regularity of self-assembling nanostructures — ●DENNIS LANGENKÄMPER, STEFAN OSTENDORP, NINA WINKLER, JÖRN LEUTHOLD, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, WWU Münster, Germany

One promising technique for fabricating large nanostructure arrays is based on Anodic Aluminium Oxide (AAO) membranes as fabrication masks or templates. With these structures it is possible to fabricate large-scale arrays of highly regular surface nano-structures including nano-particles as well as wires and tubular structures. Thereby AAO based surface nano-structuring provides an exceptional high throughput at low fabrication costs. Additionally structural parameters such as the size, shape and spacing of resulting nanostructures can be tuned by adjusting the masks' fabrication parameters. It has been shown that especially the anodization temperature and the used electrolyte and its concentration at given anodization voltage determine the properties and regularity of the AAO membrane. Our work now focuses on the impact of hydrodynamic fabrication parameters on the structures' regularity. Membranes fabricated under different hydrodynamic conditions varying in laminar and turbulent flow and flux of the respective electrolyte used during anodization have been analyzed by a computational/graphical method based on Delauney Triangulations and Voronoi Diagrams applied to high resolution SEM micrographs of the respective structures.

MM 34.20 Tue 18:00 P4

Core-shell nanoparticles from the gas phase — ●JÖRG PRIBBENOW^{1,2}, ALEXANDER SURREY^{1,3}, DARIUS POHL¹, LUDWIG SCHULTZ^{1,3}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, D-01069 Dresden, Germany — ²TU Dresden, IFWW, D-01062 Dresden, Germany — ³TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

Core-shell nanoparticles allow for the combination of different materials for the creation of systems with a wide range of functionalities. The gas-phase based preparation of such heterogeneous particles is reported here. The cores of the nanoparticles are generated by inert gas condensation in a high-pressure magnetron sputter source. While the latter is already well established, the subsequent in-flight coating of such particles with a second material by linear magnetron sputtering is a rather novel approach. Series of electrostatic lenses provide for collimation and deceleration of unipolarly charged nanoparticles in the coating chamber. The present work is focused on the preparation of particles with a molybdenum or silver core and a copper shell. Aberration-corrected high-resolution transmission electron microscopy (HRTEM) is used to investigate the local structure and chemical composition. The influence of the electrical field profile on the resulting

core-shell particles will be discussed.

MM 34.21 Tue 18:00 P4

Investigation of Nanoparticle Growth in a Dusty Acetylene Plasma — ●ALEXANDER HINZ¹, ERIK VON WAHL², MAIK FRÖHLICH², THOMAS STRUNSKUS¹, and HOLGER KERSTEN² — ¹CAU zu Kiel, Technische Fakultät, LS Materialverbunde, Kaiserstraße 2, 24143 Kiel — ²CAU zu Kiel, IEAP, AG Plasmatechnologie, Leibnizstraße 11-19, 24098 Kiel

Dusty plasmas are not only of fundamental interest but also of practical importance. Formation in plasmas is seen as a new route to prepare nanoparticles of well defined size and composition. While the particle formation in silane plasmas is well investigated it is less understood in acetylene plasmas. In particular the early stages of the particle growth are not well investigated since they are experimentally inaccessible by standard methods like Mie-Scattering. In order to get a better insight in the early stages of the particle growth a novel collection method based on neutral drag was tested. Size-distributions of the nanoparticles at different points of the growth cycle were determined ex-situ and correlated with in-situ measurement of the bias voltage of the capacitively-coupled discharge plasma. Additionally, preliminary experiments employing grazing-incidence small angle X-ray scattering (GISAXS) were performed ex-situ on the collected carbonaceous nanoparticles.

MM 34.22 Tue 18:00 P4

Crystalline structure of silver nanowires within a soft template — ●EGON STEEG, FRANK POLZER, HOLM KIRMSE, YAN QIAO, JÜRGEN P. RABE, and STEFAN KIRSTEIN — Institut für Physik, Humboldt-Universität zu Berlin

The reduction of AgNO₃ in the presence of tubular J-aggregates was used to prepare silver nanowires [1]. These wires are about 7 nm in diameter and have lengths exceeding micrometers. Within the wires single crystalline domains with length exceeding 100 nm are found by means of high resolution transmission electron microscopy (HRTEM). The structure of these domains is analyzed further by selected area electron diffraction (SAED) on single nanowires. The resulting diffraction pattern cannot be explained by the simple silver fcc lattice, although energy-dispersive X-ray spectroscopy on the wires confirms the chemical composition of silver. Different structure models are discussed taking into account stacking faults [2], internal strain, and the formation of silver complexes with organic components.

[1] D.M. Eisele et al., J. Am. Chem. Soc. 132 (2010) 2104.

[2] V. Germain et al., J. Phys. Chem. B, Vol. 107, No. 34, 2003

MM 34.23 Tue 18:00 P4

TEM investigation of segregation phenomena in Nd-Fe-B nanoparticles — ●FRANK SCHMIDT^{1,2}, DARIUS POHL¹, LUDWIG SCHULTZ¹, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — ²TU Dresden, IFWW, D-01062 Dresden, Germany

Nd₂Fe₁₄B is a comparably hard magnetic phase as L₁₀-ordered FePt, however, with a smaller Curie temperature. Therefore, Nd₂Fe₁₄B nanomagnets could be an interesting materials alternative the widely discussed L₁₀-FePt in HAMR media. There are different methods to synthesize Nd₂Fe₁₄B nanoparticles, such as chemical methods or surfactant-assisted ball milling.

The purpose of this study is to investigate free Nd-Fe-B nanoparticles prepared by inert gas condensation and how different thermodynamic conditions affect them. In-flight optical annealing of the nanoparticles allows to compare unheated particles with heated particles, which are assumed to be closer to the thermally equilibrated state. Transmission electron microscopy was used to determine the atomic structure and chemical composition of the particles. Unheated particles are found to be mainly amorphous, while rapidly optically annealed particles are crystalline. We observe both a Nd enrichment in the shell and a Fe enrichment in the core of the differently treated particles. This segregation is more pronounced for heated particles, where a clear core-shell structure is formed that can be explained by a reduction of the surface energy.

MM 34.24 Tue 18:00 P4

Transport Properties of Single TiO₂ Nanotubes — ●MARKUS STILLER¹, JOSE BARZOLA-QUIQUIA¹, ISRAEL LORITE¹, PABLO ESQUINAZI¹, ROBIN KIRCHGEORG², SERGIU P. ALBU², and PATRIK SCHMUKI^{2,3} — ¹Division of Superconductivity and Magnetism, Institute for Experimental Physics II, University of Leipzig, D-04103

Leipzig, Germany — ²Chair for Surface Science and Corrosion Department Material Science and Engineering, University of Erlangen, D-91058 Erlangen, Germany — ³Department of Chemistry, King Abdulaziz University, Jeddah, Saudi Arabia

We have investigated the electric transport properties of single TiO₂ nanotubes separated from an anodic titania nanotube array. The nanotubes have been contacted using electron beam lithography and several transport properties have been measured. The temperature dependence of the resistance, measured with the conventional four point method, of all investigated samples, show a Mott variable range hopping behavior. The results obtained with two contacts indicate the existence of a potential barrier between the Cr/Au contacts and samples surfaces, which influence is clearly observable for temperatures less than 150 K. Impedance spectroscopy in the frequency range of 40 Hz to 1 MHz carried out at room temperature, indicates that the electronic transport of these polycrystalline tubes is dominated by the grain cores.

MM 34.25 Tue 18:00 P4

Molecular dynamics simulations of morphology transitions during growth of copper nanoclusters — ●ALEXEY TAL¹, E. PETER MÜNGER¹, NILS BRENNING², IRIS PILCH¹, ULF HELMERSSON¹, and IGOR ABRIKOSOV¹ — ¹Linköping University, Linköping, Sweden — ²The Royal Institute of Technology, Stockholm, Sweden

The study of metal nanoclusters has been a subject of intense research activities in recent years. This is due to their great importance in a variety of applications. Properties of nanoclusters crucially depend on growth methods and conditions during the growth. An understanding of the growth process during the early stages is of particular interest since the morphology of the seeds may determine the structure of the final large clusters. Morphology transition of the seed should be treated as a dynamical process, a requirement is met by classical MD simulations. In principle morphology transition is determined by both, thermodynamics and kinetics. Thermodynamics tends to minimize surface energy and internal stresses. But observations of large clusters with thermodynamically unfavorable structures suggest that kinetics also plays an important role. In this study the morphology transition of clusters at an early stage is considered. The influence of the angular distributions of incoming particles is determined for Cu clusters growth from a seed with 147 atoms. It is shown that growth kinetics crucially affects the morphology transition for small clusters and forbids transition to a most favorable structure for large clusters. The temperature distribution inside the cluster during the growth is calculated and the role of temperature fluctuations is discussed.

MM 34.26 Tue 18:00 P4

Grain Refinement in Ball-Milled Nanocrystalline Iron in Dependence of its Oxygen Content — ●MARIE TRYNOGGA, CHRISTINE BORCHERS, and REINER KIRCHHEIM — Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Nanocrystalline iron-oxygen alloys with different oxygen contents were prepared by ball milling of iron and hematite (Fe₂O₃) powder for 50 hours. The composition was identified using synchrotron diffraction and atom probe tomography (APT). The samples consist mainly of α -iron, segregated oxygen and magnetite (Fe₃O₄). The microstructure was investigated by X-ray diffraction (XRD), transmission electron microscopy (TEM) and APT. We observe that the grain size decreases with increasing oxygen concentration. This is interpreted as a decrease of the grain boundary energy of iron. To examine thermal stability, differential scanning calorimetry (DSC) and synchrotron diffraction measurements were performed in-situ during heating, revealing the formation of magnetite and grain growth. The nanocrystalline structure persists at higher temperatures indicating the formation of a grain boundary phase consisting of magnetite. Above 570°C the magnetite partly transforms into wüstite (FeO). We relate our findings to the results of a previous work studying nanocrystalline iron-carbon alloys after 100 hours of ball milling [1].

[1] Y.Z. Chen, A. Herz, Y.J. Li, C. Borchers, P. Choi, D. Raabe, R. Kirchheim, Nanocrystalline Fe-C alloys produced by ball milling of iron and graphite, Acta Materialia 61:3172-3185, 2013.

MM 34.27 Tue 18:00 P4

Analysis of the pressure dependence of plasticity in nanocrystalline Pd90Au10 — ●ANJA STEINBACH, NICOLE FÈVRE, CHRISTIAN BRAUN, and RAINER BIRRINGER — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

We examine the pressure or normal stress dependence of the mechanical behavior of nanocrystalline Pd90Au10 by utilizing the miniaturized shear compression specimen (m-SCS) [1]. In this specific testing geometry, the plastic deformation caused by dominant shear stress is confined to the gauge section which is inclined at an angle α ($\alpha = 45^\circ$ for standard geometry) relative to the loading direction. Variations of the inclination angle allow varying the superimposed hydrostatic pressure in the gauge section. Based on the experimentally determined force-displacement diagram, the stress-strain-curve and further parameters like the hydrostatic pressure are calculated using FEM-simulations. On this poster we present inclination angle-dependent stress-strain-curves obtained from inert gas condensed Pd90Au10 samples with a mean grain size of 10 nm. In agreement with theory [2], we find that nanocrystalline Pd90Au10 is stronger under pressure.

[1] M. Ames, J. Markmann, R. Birringer, Mater. Sci. Eng. A 528, 526 (2010) [2] A.C. Lund, C.A. Schuh, Acta Mater. 53, 3193 (2005)

MM 34.28 Tue 18:00 P4

Solute content and structural configuration dependent mechanical properties of nanocrystalline PdAu alloys — ●NICOLE FÈVRE, CHRISTIAN BRAUN, MICHAEL DECKARM, JONAS HEPPE, ANDREAS LEIBNER, and RAINER BIRRINGER — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

We investigate elasticity and plasticity of nanocrystalline PdAu by systematically varying the Au concentration. From calorimetry we find that grain boundaries in as-prepared specimens manifest non-equilibrium configurations. Thermal annealing leads to grain boundary relaxation and so local equilibrium configurations are generated. In particular, we determine high frequency elastic moduli and Vickers hardness for as-prepared and relaxed specimens and discuss the composition-dependent evolution of strength.

MM 34.29 Tue 18:00 P4

Microstructure, Texture and Properties of severely twinned copper wires — ●ALEXANDER KAUFFMANN^{1,2}, JENS FREUDENBERGER^{1,3}, HANSJÖRG KLAUSS¹, VOLKER KLEMM³, WOLFRAM SCHILLINGER⁴, V. SUBRAMANYA SARMA⁵, and LUDWIG SCHULTZ^{1,2} — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — ²TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — ³TU Bergakademie Freiberg, Institute of Materials Science, Gustav-Zeuner-Str. 5, 09599 Freiberg, Germany — ⁴Wieland-Werke AG, Graf-Arco-Strasse 36, 89079 Ulm, Germany — ⁵Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai 600036, India

Due to the a drawing process in liquid nitrogen a drastic refinement of the microstructure of pure copper can be achieved by the activation of severe deformation twinning. In order to facilitate and enhance the refinement process an additional reduction of stacking fault energy by alloying can be applied. We are presenting the influences of severe deformation twinning on the microstructure and texture of copper and single-phase copper-aluminium alloys on the one hand and the mechanical and electrical properties on the other hand.

MM 34.30 Tue 18:00 P4

Ab-initio study of impurities diffusion in copper — ●ANTON BOCHKAREV and MAXIM POPOV — Materials Center Leoben Forschung GmbH, A-8700 Leoben, Austria

We present results of an ab initio study of impurity diffusion in bulk copper. Two types of impurities are investigated: oxygen and aluminum. The mechanisms we considered are the interstitial diffusion and the vacancy-mediated diffusion. To discover the impurity migration paths describing the elementary diffusion processes we employed the nudged elastic band (NEB) method. Arrhenius pre-factors were estimated in the framework of the transition state theory (TST). We find that oxygen is likely to diffuse through interstitials, whereas aluminum prefers vacancy-driven diffusion. The diffusivities obtained in our work are in reasonable agreement to the available experimental data.

MM 34.31 Tue 18:00 P4

effect of gap-size on phonon tunneling in Au(111)/vacuum/Au(111) — ●SAEIDEH EDALATI BOOSTAN, MICHAEL CZERNER, MICHAEL BACHMANN, and CHRISTIAN HEILIGER — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Recent experimental and theoretical investigations have shown that phonons can transport across vacuum gaps of a few angstroms wide

which called "phonon tunneling" [1,2,3]. In this work we perform ab initio calculations by using abinit software package to get interactions between atoms, which are modeled by spring constants. These interatomic force constants are used within an Atomistic Green's Function (AGF) method to calculate phonon tunneling in Au(111)/Vacuum/Au(111) system for different gap-sizes.

- [1] Igor Altfeder et al., Phys. Rev. Lett. 105, 166101 (2010)
 [2] Mika Prunnila and Johanna Meltaus, Phys. Rev. Lett. 105, 125501 (2010)
 [3] D. P. Sellan et al., Phys. Rev. B 85, 024118 (2012)

MM 34.32 Tue 18:00 P4

Calculations of Thermal Conductivity across an Interface using Beam Matching — DEBANJAN BASU¹, CYNTHIA VOLKERT², CHRISTIAN JOOSS², and PETER BLOEHL¹ — ¹Institute for Theoretical Physics, Clausthal University of Technology — ²Institute for Material Physics, University of Goettingen

Thermal conductivity is an important factor affecting the efficiency of thermoelectric devices. Our goal is to explore the thermal transmission due to phonons in multilayered structures on a mode-by-mode basis using the Beam Matching Technique. For this purpose, we determine the "complex bandstructure", which describes propagating as well as evanescent phonon modes of the individual materials of this multilayer. We describe how to extract the matching conditions from the classical equations of motion for the atoms.

MM 34.33 Tue 18:00 P4

Accessing the excitation and relaxation pathways in the ultrafast Carrier dynamics of BaSnO₃:La perovskite — KESTUTIS BUDZINAUSKAS¹, ROLF VERSTEEG¹, MATTEO MONTAGNESE¹, XUAN LUO², SANG W. CHEONG^{2,3}, and PAUL H.M. VAN LOOSDRECHT¹ — ¹II Physikalisches Institut, University of Cologne, Cologne, Germany — ²Laboratory of Pohang Emergent Materials and Department of Physics, Pohang, Korea — ³Rutgers Center for Emergent Materials and Department of Physics and Astronomy, New Jersey, USA

The Lanthanum doped Barium tin oxide BaSnO₃:La is a transparent conducting oxide (TCO). Unlike other perovskites it shows an extremely high electron mobility, reaching values up to 320 cm² V⁻¹ s⁻¹ at room temperature, making it a promising alternative to other more expensive or unstable TCO's for applications.

The microscopic mechanisms leading to such high and uncharacteristic electron mean free paths are not fully understood. We have studied the non-equilibrium carrier dynamics in the material employing ultrafast time-resolved spectroscopy in the visible, near Infrared and THz range of the optical spectrum. In this way we are able to track and elucidate the different carrier excitation and relaxation pathways in this intriguing compound.

MM 34.34 Tue 18:00 P4

Interdiffusion studies of B2 Ni-Al-Si alloys at 1173 K — DANDAN LIU^{1,2}, LIJUN ZHANG¹, YONG DU¹, SERGIY DIVINSKI², and GERHARD WILDE² — ¹State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan, 410083, PR China — ²Institute of Materials Physics, Westfälische-Wilhelms University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

The knowledge of diffusion is fundamental for the production of B2 NiAl alloys as well as their use in technological applications. In the present work, Si was added to B2 NiAl alloys, and the interdiffusion of B2 Ni-Al-Si alloys at 1173 K was investigated via the Matano-Kirkaldy method by utilizing five groups of bulk diffusion couples and the electron probe microanalysis technique. The reliability of the obtained interdiffusion data was validated by thermodynamic constraints as well as by Fick's second law applied to a numerical simulation. The results show that the presently obtained diffusivities can satisfactorily simulate the measured concentration profiles. Besides, the addition of Si was found to have different effect on the diffusion of Al in Ni-rich and nearly stoichiometric NiAl alloys. The possible reasons were interpreted in terms of cross diffusivities, site occupations, and different diffusion mechanisms. The present work provides valuable information for understanding diffusion in B2 NiAl-X alloys, where X occupies the Al sublattice.

MM 34.35 Tue 18:00 P4

Scanning Transmission Electron Tomography on three-dimensional defects in semiconductor heterostructures — MICHAEL NIEHLE and ACHIM TRAMPERT — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

Shrinking structures incorporated into opto-electronic devices require an understanding of structure-property relations on a scale of only a few nanometers. In this context, the interest in three-dimensional (3D) structures of crystal defects is growing as their detailed influence on device functionality has to be considered. The combination of scanning transmission electron microscopy (STEM) with tomography allows for an investigation of the defects' 3D structure on a respective length scale. We present the application of STEM tomography on 3D objects embedded in GaSb based semiconductor heterostructures grown on Si substrates. The unique possibility to characterize the complex morphology in great detail is demonstrated. Challenges to apply STEM tomography as a routine tool in materials sciences are discussed with respect to materials comprising elements with a rather high atomic number. Strategies to complement investigations by conventional TEM techniques are sketched.

MM 34.36 Tue 18:00 P4

Lateral Resolved EELS on organic bulk heterojunctions - a low-dose approach to optimized spatial and energy resolution in the TEM — ANNE K. KAST^{1,2,3}, MARTIN PFANMÖLLER¹, MARCO OSTER¹, PHILIPP WACHSMUTH⁴, RALF HAMBACH⁴, GERD BENNER⁵, DIANA NANOVA^{2,3}, ROBERT LOVRINCIC^{2,3}, WOLFGANG KOWALSKY^{2,3}, UTE KAISER⁴, and RASMUS R. SCHRÖDER^{1,3} — ¹Cryo-EM, Universitätsklinikum Heidelberg — ²IHF, TU Braunschweig — ³innovationLab GmbH, Heidelberg — ⁴Materialwissenschaftliche EM, Uni Ulm — ⁵Carl Zeiss GmbH, Oberkochen

We implement a novel analytical method using EFTEM which allows visualizing donor and acceptor materials in organic solar cell thin films by analyzing electronic excitations features in the optical and plasmonic energy region. Segmentation by EELS reveals that these carbon based materials show characteristic optical excitations in energy-loss spectra. However, the blend materials are very sensitive to radiation damage, which impedes spatial spectral mapping using EELS in conventional scanning beam mode. We introduce an automated scheme that exploits the inherent spatial resolution in the EEL spectrum as it is obtainable from aberration corrected imaging energy filters. It involves automatic scanning of the image of a slit aperture in the illumination beam path. To eliminate residual image distortion in the EEL spectrum we apply correction algorithms for quantitative spectrum interpretation. Application of such automated laterally resolved EEL spectroscopy allows spatial mapping of high-resolution spectra in two dimensions at low-dose conditions.

MM 34.37 Tue 18:00 P4

STEM with focused vortex beams - a route towards local EMCD measurements? — DARIUS POHL¹, SEBASTIAN SCHNEIDER^{1,2}, LUDWIG SCHULTZ^{1,2}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — ²TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

X-ray magnetic circular dichroism is a well established method to study element specific magnetic properties of a material, while electron magnetic circular dichroism (EMCD), which is the electron wave analogue to XMCD, is scarcely used today. Recently discovered electron vortex beams, which carry a discrete orbital angular momentum (OAM) L, are predicted to also reveal dichroic signals. Since electron beams can be easily focused down to sub-nanometer diameters, this novel technique provides the possibility to quantitatively determine local magnetic properties with unrivalled lateral resolution. As the spiralling wave front of the electron vortex beam has an azimuthally growing phase shift of up to 2π and a phase singularity in its axial center, specially designed apertures are needed to generate such non-planar electron waves. We report on the preparation and successful implementation of spiral apertures into the condenser lens system of an aberration-corrected FEI Titan³ 80-300 transmission electron microscope (TEM). This setup allows to perform scanning TEM (STEM) with vortex beams carrying user-selected OAM. First experiments and simulations on the interaction of the vortex beam with a crystalline sample will be presented.

MM 34.38 Tue 18:00 P4

Combined experimental and theoretical study showing D1_a-type local order in Ni-Re — SASCHA B. MAISEL¹, NILS SCHINDZIELORZ¹, ALESSANDRO MOTTURA², ROGER REED³, and STEFAN MÜLLER¹ — ¹Institute of Advanced Ceramics, TUHH, 21073 Hamburg, Deutschland — ²School of Metallurgy and Materials, University of Birmingham, B15 2TT Edgbaston, United Kingdom —

³Department of Engineering Science, University of Oxford, OX1 3PJ Oxford, United Kingdom

Since the 1980s rhenium has been used as an addition to nickel-based high-temperature superalloys, since even small amounts of rhenium have a dramatic effect on creep resistance. However, the mechanisms behind this so-called *rhenium-effect* are still ill-understood. Using both experimental and theoretical methods, we show that the currently known phase diagram is inaccurate, and neglects a stoichiometric compound at 20 at.% Re Ni₄Re. This is expected to affect the microstructure of Ni-Re alloys, with important ramifications for Ni-based superalloys. The Ni₄Re compound is shown to be stable by means of quantum mechanical high-throughput calculations at 0K, aided by the cluster-expansion methods. Monte Carlo simulations show that it is thermally persistent up to 1100 K when considering configurational entropy. The existence of this compound was experimentally confirmed using extended x-ray absorption fine spectroscopy on a Ni₉₇Re₀₃ alloy.

MM 34.39 Tue 18:00 P4

A synchrotron analysis of deformation-induced martensitic transformation in the as-cast Cu₄₀Co₁₀Zr₅₀ — ●FATEMEH A. JAVID^{1,2}, NORBERT MATTERN¹, JOZEF BEDNARCIK³, MOHAMMAD SIAHATGAR⁴, MIHAI STOICA¹, SIMON PAULY¹, and JÜRGEN ECKERT^{1,2} — ¹Leibniz Institute for Solid State and Materials Research, Dresden, Germany — ²Technische Universität, Dresden, Germany — ³DESY, Forschungsbereich FS, Hamburg, Germany — ⁴Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

The deformation-induced martensitic transformation in Cu₄₀Co₁₀Zr₅₀ alloy under mechanical load was investigated using a synchrotron X-ray diffraction. The *in-situ* compression tests were performed in both track control and load control modes. The X-ray diffraction results show that the position of the diffraction peaks shifted to higher *q* values (reciprocal space) and peaks broaden due to increasing of strain. Considering

the phase transformation fractions, the kinetics of phase transformation was studied in the longitudinal and transversal directions. In the case of track control test, the measured *B2* (Cu,Co)Zr→M(Cu,Co)Zr transformation fractions indicates a 100% of martensitic transformation under compression loading and the microstructure consists of a fully martensitic (Cu,Co)Zr. Whilst upon load control test, the martensitic transformation occurred > 90%. The changes in the strain tensor and subsequently the shear components versus applied stress were studied.

MM 34.40 Tue 18:00 P4

Dependence of accessible undercooling on prior liquid overheating by differential fast scanning calorimeter — ●BIN YANG¹, JOHN H. PEREPEZKO², JÜRGEN W. P. SCHMELZER¹, YULAI GAO³, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Department of Materials Science and Engineering, University of Wisconsin-Madison, 1509 University Avenue, Madison, WI 53706, USA — ³School of Materials Science and Engineering, Shanghai University, Shanghai 200072, P.R. China

The dependence of accessible undercooling on prior overheating of a pure tin single micron-sized droplet was studied by differential fast scanning calorimetry (DFSC) with cooling rates from 500 to 10,000 K/s. It is observed experimentally that (i) the degree of undercooling increases first gradually with increasing of prior overheating and reaches then an undercooling plateau; (ii) the accessible undercooling increases initially with increasing cooling rate. However, above a certain cooling rate the accessible undercooling decreases strongly with increasing cooling rate. For overheating levels above that for the onset of the undercooling plateau the undercooling increases with increasing cooling rate. These observed unusual behavior is successfully explained by heterogeneous nucleation in cavities. This mechanism can possibly also describe nucleation in other similar rapid solidification processes.

MM 35: Invited Talk (Hauptvortrag) Spatschek

Time: Wednesday 9:30–10:00

Location: BAR 205

Invited Talk MM 35.1 Wed 9:30 BAR 205
From grain boundary premelting to liquid metal embrittlement: A modelling perspective — ●ROBERT SPATSCHEK — Max-Planck Institut für Eisenforschung, Düsseldorf

The embrittlement of a polycrystalline ductile metal by the attack of a lower melting point metal is a long-standing problem for many industrial applications, and it has often led to disastrous material failure. Despite significant progress in understanding, the complexity of mechanisms involved and their interplay make a profound comprehension of this effect very challenging.

In this talk I will focus on a specific aspect of the embrittlement process, which is related to the phenomenon of grain boundary premelting. It allows for the formation of thin liquid films at grain boundaries al-

ready below the bulk melting point, which therefore facilitates fast transport of alloying components in a polycrystalline material with simultaneous reduction of strength. Recent developments of amplitude equations models allow to address this phenomenon from a theoretical and modelling perspective, linking continuum aspects of phase formation with the atomistic features of grain boundaries. This model allows to explain quantitatively the grain boundary premelting transition in terms of a short ranged interaction between adjacent solid-melt interfaces.

Beyond the analysis of nanoscale equilibria, also the kinetics of the grain boundary wetting process will be discussed, using a new Green's function based description. We find that the short ranged interactions strongly influence the wetting kinetics in the diffusion-limited regime.

MM 36: Topical Session: Thermodynamics at the nano scale IV - Electrochemistry and strain

Time: Wednesday 10:15–11:45

Location: BAR 205

Topical Talk MM 36.1 Wed 10:15 BAR 205
First-principles prediction of the equilibrium shape of nano particles under realistic electrochemical conditions — ●NICOLA MARZARI¹ and NICEPHORE BONNET² — ¹Theory and Simulations of Materials, EPFL — ²AIST and University of Tokyo

A first-principles model of the electrochemical double layer is applied to study surface energies and surface coverage under realistic electrochemical conditions and to determine the equilibrium shape of metal nanoparticles as a function of applied potential. The potential bias is directly controlled by adding electronic charge to the system, while total energy calculations and thermodynamic relations are used to predict electrodeposition curves and changes in surface energies and coverage. This approach is applied to Pt surfaces subject to hydrogen underpotential deposition. The shape of Pt nanoparticles under a cathodic scan is shown to undergo an octahedric-to-cubic transition, which is more pronounced in alkaline media due to the interaction

energy of the pH-dependent surface charge with the surface dipole.

References: N. Bonnet and N. Marzari, Phys. Rev. Lett. 110. 086104 (2013).

MM 36.2 Wed 10:45 BAR 205

Calculation of pourbaix diagrams combining DFT and experimental data as descriptor for high-throughput screening — ●IVANO E. CASTELLI, KRISTIAN S. THYGESEN, and KARSTEN W. JACOBSEN — Technical University of Denmark, Kgs. Lyngby, Denmark
Stability is the most important criterion for a material to be used in any type of application. It is often calculated relative to experimentally known structures in which the candidate material can separate. This method gives no information about corrosion in water. Stability in a realistic electrochemical environment can be investigated using Pourbaix diagrams that combine experimental information, namely dissolution energies, with computational data from density functional

theory (DFT) total energies [1].

With this approach, the stability in water of 20 cubic perovskites previously screened for one-photon water splitting device [2] has been investigated. These materials are usually stable at $\text{pH} = 7$ and $U = 0$ V. Oxides and oxyfluorides are also stable at high potential, while oxynitrides at low potential [3].

Furthermore, the stability in water is efficiently used as a descriptor, together with size and position of the bandgap, for high-throughput screening for energy related applications of known materials from the Materials Project database [4,5].

References [1] K.A. Persson et al., *Phys Rev B* 85, 235438 (2012). [2] I.E. Castelli et al., *Energy Environ. Sci.* 5, 5814 (2012); *Energy Environ. Sci.* 5, 9034 (2012). [3] I.E. Castelli et al., *Topics in Catalysis* (2013). [4] <http://materialsproject.org/> [5] <https://cmr.fysik.dtu.dk/>

Topical Talk

MM 36.3 Wed 11:00 BAR 205

Interface stress effects and critical behavior in nanocrystalline materials — ●RAINER BIRRINGER — Universität des Saarlandes, Saarbrücken

We discuss the concept of interface stress in nanocrystalline (nc) materials made up of grain- and/or phase boundaries. Interface stress is an inherent property of any interfacial material manifesting solid-solid or solid-liquid interfaces. In nc metals the stress exerted by interface stress on the abutting crystallites scales as one over grain size and may assume values of the order of several GPa in the limit of small grain sizes. We present data for grain boundary stress in noble metals and address the issue of interface stress at the Ni-Ag phase boundary.

The critical behavior at the para- to ferromagnetic phase transition is usually considered not being dependent on the microstructural details of the system but depends only on the respective universality class, the dimensionality of the space and the symmetry of the order

parameter. We studied nc Gadolinium to scrutinize whether or not the randomness and disorder associated with nanocrystallinity may act as a relevant scaling field and so make the system change its universality class, derived from the single crystalline state, when approaching the asymptotic critical regime in the limit of small grain sizes.

MM 36.4 Wed 11:30 BAR 205

Surface excess elasticity in nanostructures: fact or fiction? — ●NADIA MAMEKA¹, JÜRGEN MARKMANN^{1,2}, and JÖRG WEISSMÜLLER^{1,2} — ¹Helmholtz-Zentrum Geesthacht, Institut für Werkstofforschung, Werkstoffmechanik, Geesthacht, Germany — ²Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, Hamburg, Germany

Solid surfaces interact with the underlying bulk via a capillary force, the surface stress, which varies as the solid is strained. This variation defines a surface excess elastic modulus, which is well documented in theory. For nanoscale structures, the excess elasticity implies a size-dependent effective elastic response of the entire structure. While experimental observations of this phenomenon have been claimed, no agreement has been reached about magnitude or even sign of the excess modulus. One may therefore ask if there is a measurable impact at all. Here, we use experiments with dynamic mechanical analysis (DMA) on nanoporous gold to probe the issue. We focus on reversible changes in the elastic response when the surface is electrically charged or adsorbate monolayers deposited and lifted in electrolyte. The results reveal a significant variation in macroscopic stiffness. This conclusively confirms the important role of the surface excess elasticity phenomena in materials with large specific surface area. As an example, the reversible variation of the elastic modulus in the presence of weakly binding ClO_4^- ions to the Au surface reached up to 10% for a ligament size of 40 nm in mm-sized samples.

MM 37: Computational Materials Modelling V - Point defects

Time: Wednesday 10:15–11:15

Location: IFW D

MM 37.1 Wed 10:15 IFW D

Solute-vacancy interaction and diffusion of selected elements in Ni-based superalloys. — ●SERGEJ SCHUWALOW, JUTTA ROGAL, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

The dependence of high-temperature properties of Ni-based superalloys on the alloying additives is a subject of ongoing research. Current knowledge is mostly phenomenological in nature and the details of solute diffusion, interaction with defects such as interfaces, vacancies, and dislocations as well as the interplay between composition and microstructure are not well understood.

In this work we investigate the solute-vacancy interactions and concentration/temperature-dependent diffusion behavior of selected alloying elements using a combination of density-functional theory calculations and kinetic Monte Carlo simulations.

Vacancy mobility is found to be only weakly influenced by solute presence, even for heavy refractory elements such as Re. Diffusion coefficients calculated by our approach are shown to be in good agreement with both experiment and simpler, but more limited, analytic models.

MM 37.2 Wed 10:30 IFW D

Effect of Fe and Cu doping on properties of TiNi Alloys — ●MARTIN ZELENÝ^{1,2}, XIANGQIAN YIN², and XUJUN MI² — ¹Institute of Materials Science and Engineering, NETME Centre, Brno University of Technology, Brno, Czech Republic — ²General Research Institute for Nonferrous Metals, Beijing, P. R. China

The effect of Fe and Cu on the martensitic transformation behavior and mechanical properties of TiNi alloys has been investigated by calculating of the lattice constants and elastic moduli of the B2 phase. The site preference for both doping elements has been studied as well. The calculations were performed using the coherent potential approximation implemented within the framework of the exact muffin-tin orbitals method. Our theoretical results show contraction of the lattice constant of TiNi with increasing concentration of Fe. Added Fe atoms will always occupy the Ni sublattice even in the alloys where Ti is in deficiency. On the other hand added Cu atoms will occupy the sublattice of element in deficiency. This result has been also confirmed

by our XRD measurements.

The calculated elastic constants allow us to predict the martensitic transformation temperature, because this temperature is correlated with the C_{44} elastic constant. The composition dependence of elastic moduli and stability of B2 structure is discussed on the basis of the electronic density of states and phonon density of states.

MM 37.3 Wed 10:45 IFW D

Sublattice solubility of transition metals in L1₂ phases in Co-based superalloys — ●JÖRG KOSSMANN¹, THOMAS HAMMERSCHMIDT¹, SASCHA MAISEL², STEFAN MÜLLER², and RALF DRAUTZ¹ — ¹ICAMS, Ruhr-University Bochum, Bochum, Germany — ²Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Superalloys are a class of advanced materials that are used e.g. to cast turbine blades for aircraft engines because of their good mechanical stability even at high temperatures. They owe their high-temperature toughness to hardening by precipitation of γ' particles (L1₂ structure) which coexist with the coherent γ phase (disordered fcc). Since Sato *et al.* first observed a L1₂ phase in the ternary Co-Al-W system, Co-based materials have been shown to be promising candidates for the next generation of superalloys. We investigate the solubility of the transition metals (TM) W, Mo, Cr, Ti, and Ta in L1₂-Co₃(Al_xTM_{1-x}) with density functional theory calculations. For the description of the sublattice disorder we use the cluster expansion and special quasi-random structures. This work is part of the collaborative research center SFB/TR 103.

MM 37.4 Wed 11:00 IFW D

Vacancies in fcc metals — ●MOSTAFA MORTAZAVIFAR and MARTIN OETTEL — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Tübingen, Germany

Through a cluster expansion of the crystal partition function, we derive an approximate expression for the equilibrium concentration of thermal vacancies in solids which allows for a transparent interpretation of the vacancy volume and the energetic/entropic part in the corresponding Gibbs energy of vacancy formation ΔG_v . For the text-book model crystals made of hard spheres and Lennard-Jones particles very good agreement with simulation data is found. Application to Ni through

the embedded-atom method (EAM) reveals a strong sensitivity of the variation of ΔG_v with temperature to details of the EAM potential [1]. We propose to use our formula for $\Delta G_v(T)$ in reference calculations where the needed partition function terms should be evaluated by quantum density functional theory (qDFT). The results can be em-

ployed in theoretical materials science using ab-initio methods or in constructing effective classical potentials.

[1] M. Mortazavifar and M. Oettel, *Thermal vacancies in close-packing solids*, arXiv:1311.5093 [cond-mat.soft]

MM 38: Structural materials

Time: Wednesday 10:15–11:45

Location: IFW B

MM 38.1 Wed 10:15 IFW B

Relation between thermodynamic stability and stacking fault energies in Mg alloys: An ab-initio study — ●ZONGRUI PEI^{1,2}, LI-FANG ZHU¹, MARTIN FRIÁK¹, STEFANIE SANDLÖBES¹, STEFAN ZAEFFERER¹, BOB SVENDSEN^{1,2,3}, DIERK RAABE¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Germany — ³Faculty of Georesources and Materials Engineering, RWTH Aachen University, Germany

Pure magnesium and most commercial wrought magnesium alloys exhibit a low room temperature ductility which can be significantly increased by the addition of Y or rare earth (RE) elements (Acta Mater. 59 (2011) 429). Understanding the mechanisms causing this ductility enhancement on an atomistic and electronic-structure level would provide a systematic approach to identify alternative favorable solutes. Therefore, in order to obtain a deeper insight into the mechanisms active in the Mg-Y and Mg-RE alloys, an ab-initio study of the compositional dependence of intrinsic stacking fault (ISF) energies have been performed. Employing density functional theory (DFT) calculations, the ISF energies have been determined within the Axial Next-Nearest-Neighbour Ising (ANNI) model. An in-depth analysis of the theoretical data shows reduced ISF energies as a direct consequence of the dramatically reduced thermodynamic stability of hexagonal Mg-Y solid solutions when the Y concentration approaches its solubility limit in Mg (Acta Mater. 60 (2012) 3011).

MM 38.2 Wed 10:30 IFW B

The effect of extreme uniaxial and biaxial loading conditions in transition-metal disilicides: an ab initio study — DOMINIK LEGUT¹, ●MARTIN FRIÁK^{2,3,4}, MOJMÍR ŠOB^{4,3,5}, and JÖRG NEUGEBAUER² — ¹Nanotechnology Centre & IT4Innovations, VSB-Technical University of Ostrava, Ostrava, Czech Republic — ²Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ³Institute of Physics of Materials, AS CR, v.v.i. Brno, Czech Republic — ⁴Central European Institute of Technology (CEITEC MU), Masaryk University, Brno, Czech Republic — ⁵Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Transition-metal disilicides constitute a promising basis for a new generation of high-temperature structural materials that can significantly improve the thermal efficiency of energy conversion systems and advanced engines. Although they have been studied quite intensively, the complexity of their mechanical behavior is still not completely understood. Employing first-principles (ab initio) calculations of electronic structure, we investigate the effect of uniaxial loading for disilicides with hexagonal C40 structure, namely for NbSi₂, CrSi₂, VSi₂ and TaSi₂, and compare their behavior with previously studied C11_b structure disilicides. Further, the C40 structure disilicides are subjected to biaxial loading and the values of strains are extended up to their extreme levels, beyond materials stability limits represented here by the values of theoretical tensile strength. We find a direct correspondence between the electronic structure characteristics and the onset of strength instability.

MM 38.3 Wed 10:45 IFW B

High Strength Light-Metal composites — ●JULIANE SCHARNWEBER¹, JAN ROMBERG², ANDY ESCHKE¹, CARL-GEORG OERTEL¹, TOM MARR², JENS FREUDENBERGER², LUDWIG SCHULTZ², ILYA OKULOV², UTA KÜHN², JÜRGEN ECKERT², and WERNER SKROTZKI¹ — ¹Institut für Strukturphysik, Technische Universität Dresden, D-01062 Dresden, Germany — ²Leibniz-Institut für Festkörper- und Werkstofforschung, D-01171 Dresden, Germany

Ti/Al laminated sheets were produced by accumulative roll bonding (ARB) at ambient temperature. Intermediate annealing was found to

be suitable to overcome the issue of layer-crossing shear band formation usually observed for comparable metal combinations. This treatment resulted in composite sheets of technically relevant size with layer stability down to thicknesses of about 2 *m. The microstructure and local texture was characterized by scanning electron microscopy combined with electron backscatter diffraction, while the global texture was measured by neutron diffraction. Strength and ductility were measured in tension. The evolution of microstructure, texture and strength is described and discussed with regard to number of ARB cycles and annealing temperature. Additionally, the formation of intermetallic phases at the interfaces is addressed.

MM 38.4 Wed 11:00 IFW B

Delta' precipitation in Al-Cu-Li alloys — ●PASCAL NEIBECKER¹, HAIDER FERDINAND¹, and AL-KASSAB TALA'AT² — ¹University of Augsburg, Augsburg, Germany — ²King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Due to their high strength, high Young's modulus and low density, Al-Cu-Li alloys are of special interest in aerospace applications. The process mainly responsible for the excellent mechanical properties of these alloys is precipitation hardening. Understanding the microstructure evolution upon artificial aging of Al-Cu-Li alloys and the corresponding underlying mechanisms is thus of great importance. In mechanically untreated binary Al-Li and ternary Al-Cu-Li alloys with a high Li content, the major hardening phase is the metastable delta' (Al₃Li) phase which already partly develops during natural aging of the alloy. The formation mechanism leading to delta' precipitation thereby was controversially discussed in the last decades.

This work investigates the kinetics of the delta' evolution in an Al-1.7 at. % Cu- 5.6 at. % Li model alloy upon artificial aging at 160 °C with Differential Scanning Calorimetry and Atom Probe Tomography. Here, the volume fraction and size evolution of the delta' phase is determined and additionally, by using the Pearson coefficient, quantitative statements about Li and Cu ordering in the alloy are made. The findings give insights into the formation mechanism of the delta' phase in Al-Cu-Li alloys.

MM 38.5 Wed 11:15 IFW B

High-temperature interactions of liquid aluminum with titanium diboride ceramic — ●LIXIA XI¹, RAFAL NOWAK², IVAN KABAN^{1,3}, BARTŁOMIEJ KORPALA², GRZEGORZ BRUZDA², NATALIA SOBCZAK², NORBERT MATTERN¹, and JÜRGEN ECKERT^{1,3} — ¹IFW Dresden, Institute for Complex Materials, P.O. Box 270116, 01171 Dresden, Germany — ²Foundry Research Institute, Center for High-Temperature Studies, Zakopianska Str. 73, 30-418 Cracow, Poland — ³TU Dresden, Institute of Materials Science, 01062 Dresden, Germany

Temperature-dependent interactions in the liquid Al/TiB₂ ceramic system has been investigated by the sessile drop technique in the temperature range from 700 to 1400 C. The microstructure of the Al/TiB₂ interfaces in the solidified couples after sessile drop tests has been characterized by scanning electron microscopy, coupled with an energy-dispersive X-ray spectroscopy and X-ray diffraction. Up to about 800 C, pure Al exhibits rather poor wetting and a weak reactivity with TiB₂ ceramic; only few titanium aluminate particles were found to be formed at the interface. Starting from 800 C, the wetting improves either with time or upon further heating. Above 1000 C liquid Al completely spreads over the ceramic and penetrates along the TiB₂ grain boundaries or into the pores. Al₃Ti and Al₂O₃ were found to precipitate at the interface.

MM 38.6 Wed 11:30 IFW B

Structural analysis of dissimilar Al-Ti FSW joints — ●ROLAND MARSTATT¹, MARKUS KRUTZLINGER², MAXIMILIAN GNEDEL¹, FERDINAND HAIDER¹, and MICHAEL F. ZAEH² — ¹Lehrstuhl fuer Experimentalphysik I, Universitaet Augsburg, Augsburg, Germany — ²Institut

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 high quality joints can be produced with a minimum of deleterious intermetallic phases. Due to the process conditions, FSW seems to be a good choice to form dissimilar joints as e.g. between aluminium and titanium alloys. However, a comprehensive description of the effective joining mechanisms of friction stir welded dissimilar material joints -

formation of metallic bonds vs. interlocking mechanisms - is still a subject of research.

In this study first results of the analysis of the effects on the structure of the weld seam caused by stirring material flow are presented. FSW-joints of aluminium and titanium alloys in lap joint configuration have been investigated under varying process conditions. The results seem to show a transport of Ti into Al, which leads to considerable solid solution hardening close to the weld seam. But until now, no indication for the formation of brittle intermetallic phases has been found. Furthermore, the thermal stability of the joint with possible formation of intermetallic phases and subsequent embrittlement was studied.

MM 39: Liquid and Amorphous Metals I - Shearbands

Time: Wednesday 10:15-11:30

Location: IFW A

MM 39.1 Wed 10:15 IFW A

Kinetics of single shear bands in Zr-based bulk metallic glasses — ●PETER THURNHEER¹, ROBERT MAASS², STEFAN POGATSCHER¹, ALIREZA SAEED-AKBARI¹, and JÖRG F. LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, 8093 Zürich, Switzerland — ²Nanoskalige Materialien, Institut für Materialphysik, Georg-August Universität Göttingen, 37077 Göttingen, Germany

Mechanical properties of bulk metallic glasses are generally assessed by compression testing. However, quantities such as plasticity or the material's ability to strain-harden are often modified by geometric effects. These include initiation of constrained shear bands at sample corners and shear-band arrest at contact points between emerging shear-offsets and the cross-heads of the machine. To study freely propagating shear bands, the compression samples are equipped with a small notch, which promote the initiation of a single, major shear band well off the sample corners. In this work, we present results on the compositional dependence of single-shear-band dynamics for a set of Zr-based bulk metallic glasses, and review recent theories and experiments on shear-band propagation modes.

MM 39.2 Wed 10:30 IFW A

Mechanical analysis of amorphous solids with large amplitude oscillatory spectroscopy (LAOS) — ●STEFANIE FINKHÄUSER¹, RANKO RICHERT², CARSTEN MAHN¹, and KONRAD SAMWER¹ — ¹Physikalisches Institut, Georg-August Universität Göttingen — ²Department of Chemistry & Biochemistry, Arizona State University

In the presence of mechanical fields, glassy materials are known to reveal many interesting phenomena. One of them is a crossover from a linear behavior in stress-strain dependency to a nonlinear behavior. To investigate this crossover in detail, we use dynamic mechanical excitation with large amplitudes. The sample is excited with a sinusoidal stress whose amplitude is large enough to lead to nonlinear strain-responses. The Fourier-analysis of these nonlinear responses contains higher harmonic contributions. These can give further insight into interactions among local plastic events, which lead to the nonlinear response. By switching between large amplitudes and small amplitudes which give a linear strain-response, the time dependence of these interactions is investigated. We will show results on PMMA and bulk metallic glasses.

Financial support by the DFG SFB 937 is thankfully acknowledged.

MM 39.3 Wed 10:45 IFW A

Diffusion in shear bands of a Pd40Ni40P20 bulk metallic glass — ●ISABELLE BINKOWSKI, SERGIY V. DIVINSKI, and GERHARD WILDE — 1- 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 received increasing attention. Metallic glasses exhibit mechanical properties such as high strength and hardness, however, this advantage is impeded by the

fact that their plasticity appears to be extremely limited. The plastic deformation is localized in thin regions, called shear bands, with widths from 10nm to 50 nm, whose extension lead to catastrophic failure. Despite their obvious importance, there exist several open issues concerning the initiation, propagation, kinetics and general comprehension of shear banding. In the present study, the characteristics of shear bands in a Pd40Ni40P20 bulk metallic glass are investigated more precisely utilizing the radiotracer technique to measure atomic transport in shear bands. Additionally, combining these experimental results with calorimetric measurements should get insight into the time-dependence and the impact of structural changes on diffusion.

MM 39.4 Wed 11:00 IFW A

Elastic Susceptibility measurements of Zr-based Bulk Metallic Glass at Ultra Low Temperatures — ●MARIUS HEMPEL, ANDREAS REISER, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, 69120 Heidelberg

Many low temperature properties of glasses can be described by the standard tunnelling model. Dielectric and metallic glasses in the superconducting state far below T_C ought to yield similar results since their behaviour is solely governed by interactions between tunnelling systems and phonons in the absence of conduction electrons. We present experimental results of both temperature and frequency dependence of the internal friction and sound velocity of the bulk metallic glass $Zr_{55}Cu_{30}Al_{10}Ni_5$ which differ systematically from predictions. In particular, the observed temperature dependency of the internal friction is significantly weaker than predicted by the standard tunnelling model, but agrees reasonably well with the behaviour of thin ribbon samples of metallic glasses reported by other authors.

MM 39.5 Wed 11:15 IFW A

Boson peak in the heat capacity of severely deformed metallic glass — JONAS BÜNZ¹, ●TOBIAS BRINK², KOICHI TSUCHIYA³, GERHARD WILDE¹, and KARSTEN ALBE² — ¹Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — ²Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — ³National Institute of Materials Science, Sengen, Tsukuba, Japan

Heat capacity measurements on amorphous materials reveal an additional contribution to the low temperature heat capacity compared to crystalline materials. This so called boson peak, which is due to additional vibrational modes, appears as an excess heat capacity compared to the Debye T^3 -law. We show the influence of deformation and annealing on the boson peak of Cu-Zr-based metallic glass using differential scanning calorimetry. To elucidate the origin of the changes of boson peak intensity, we utilize molecular dynamics computer simulations and the harmonic approximation. The results indicate that the emergence of shear bands and their gradual relaxation upon annealing strongly influence the intensity of the boson peak for the whole sample. Moreover, the annealing experiments also give new insights into the thermal relaxation behavior of shear bands in metallic glasses.

MM 40: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV (O with HL/TT/MM)

Time: Wednesday 10:30–13:15

Location: TRE Ma

Topical Talk MM 40.1 Wed 10:30 TRE Ma
From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices — ●IMMANUEL BLOCH — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Ultracold atoms in optical lattice form an ideal testbed to probe the non-equilibrium dynamics of quantum many-body systems. In particular recent high-resolution imaging and control techniques allow to probe dynamically evolving non-local correlations in an unprecedented way. As an example, I will focus in my talk on the dynamical excitation of spatially ordered Rydberg structures that are formed through laser excitation from ground state Mott insulating atoms. In addition, I will show how single-spin and spin-pair impurities can be used to directly reveal polaron dynamics in a strongly interacting superfluid or the bound state of two magnons in a Heisenberg ferromagnet - a problem discussed first theoretically more than 80 years ago by H.A. Bethe. New atom interferometric schemes to directly probe the Green's function of a many-body system through the impurity dynamics will be discussed.

MM 40.2 Wed 11:00 TRE Ma
Correlated Light-Matter Interactions in Cavity QED — ●JOHANNES FLICK¹, HEIKO APPEL¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In the electronic structure community, the quantized nature of the electrons is usually (approximately) incorporated, whereas the electromagnetic field is mostly treated classically. In contrast, in quantum optics, matter is typically simplified to models with a few levels, while the quantized nature of light is fully explored. In this work, we aim at treating both, matter and light, on an equal quantized footing.

We present exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical one- or two-dimensional high-Q cavities and coupled to the quantized electromagnetic modes in the dipole or quadrupole coupling regime. We focus on spontaneous emission, strong-coupling phenomena, dipole-dipole couplings including van-der-Waals interactions, and Förster resonance energy transfer (FRET), all beyond the rotating-wave approximation.

This work has implications for a future development of a time-dependent density functional theory formulation of QED [1,2] for correlated multi-photon configurations.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).

[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

MM 40.3 Wed 11:15 TRE Ma
Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons — ●CAMILLA PELLEGRINI¹, JOHANNES FLICK², HEIKO APPEL², ILYA V. TOKATLY^{1,3}, and ANGEL RUBIO^{1,2} — ¹Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastián, Spain — ²Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — ³IKERBASQUE, Bilbao, Spain

In a recent paper [1] time dependent density functional theory has been generalized to many-electron systems strongly coupled to quantum electromagnetic modes of a microcavity. Here we construct an approximation for the corresponding exchange-correlation (xc) potential by extending the optimized effective potential (OEP) method to the electron-photon system. The derivation of the OEP equation employing the non-equilibrium Green's function formalism, and the first order approximation for the electronic self-energy is presented. Beyond the mean field level, the electron-photon coupling generates a time non-local photon-mediated interaction between the electrons, whose propagator enters the exchange-like diagram. We further show the approximated xc-potential for a model two-level diatomic molecule with one electron coupled to photon modes. The comparison between the

obtained results and the exact numerical ones in the different coupling regimes (from weak up to ultra-strong) is discussed. [1] I.V. Tokatly, Phys. Rev. Lett. **110**, 233001(2013)

MM 40.4 Wed 11:30 TRE Ma
Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics — ●HEIKO APPEL¹, JOHANNES FLICK¹, RENE JESTAEDT¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Experimental progress in recent years has enabled the fabrication of Fabry-Perot resonators with high optical quality factors (high-Q). Such cavities allow to study the interaction of matter with a quantized light field at the single-photon level (Nobel prize 2012). In this talk we present the real-time evolution of correlated photon-electron wavefunctions in optical one- and two-dimensional high-Q cavities. We discuss implications for a multi-component density functional theory for Quantum Electrodynamics [1,2] based on the time-dependent electron density and the photon energy density.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).

[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

MM 40.5 Wed 11:45 TRE Ma
Photoelectron driven plasmaron excitations in (2x2)K/Graphite — ●BO HELLSING — Department of Physics, Gothenburg University, Sweden

A new type of plasmarons formed by the compound of photoelectrons and acoustic surface plasmon (ASP) excitations is investigated in the system p(2 × 2)-K/Graphite. The physics behind these types of plasmarons, e-plasmarons, is different from the ones recently found in graphene and quantum well systems, where the loss features result from the photohole-plasmon interaction in the material, h-plasmarons. Based on the first principles scheme, Time dependent density functional (TDDFT), we calculated the linear response due to the presence of the escaping photo-electron and determine the ASP dispersion. The coupling between the photoelectron and the ASP gives rise to excitation of the e-plasmarons manifested by a broad dispersive feature shifted about 0.5 eV below parabolic K induced quantum well band (QWB) in agreement with the ARPES experiment by Agdal et al. The e-plasmarons should be considered as a source of the loss satellite structure in ARPES for 2D systems. In addition they are important to take into account in theoretical studies of different compounds as they reflect an additional channel for excitations of plasmons. This could then increase the photon-plasmon conversion yield which obviously is of interest in the field of plasmonics.

MM 40.6 Wed 12:00 TRE Ma
Charge-transfer excitations in organic systems from many-body perturbation theory — ●XAVIER BLASE¹, CARINA FABER^{1,2}, PAUL BOULANGER¹, CLAUDIO ATTACALITE¹, and IVAN DUCHEMIN² — ¹Institut Néel, CNRS and UJF, Grenoble, France — ²L.SIM/INAC, CEA, Grenoble, France

Charge-transfer excitations in organic systems lies at the heart of a large variety of physical phenomena, from photosynthesis to photovoltaics, photocatalysis or DNA denaturation. From a theoretical point of view, such nonlocal excitations are well known to lead to difficulties within the TDDFT framework, leading to the development of range-separated hybrids. We present here the merits of the Bethe-Salpeter formalism and demonstrate its ability to reproduce *cold* and *hot* Frenkel or charge-transfer excitations with remarkable accuracy [1-3]. Our calculations are based on a recent Gaussian basis implementation of the GW and Bethe-Salpeter formalism, the Fiesta initiative [1-4], allowing all-electron or pseudopotential excited states calculations for systems comprising several hundred atoms. Recent developments towards discrete and continuous embedding techniques within the many-body perturbation framework will be presented.

References: [1] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, **86**, 155315 (2012). [2] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. **109**, 167801 (2012). [3] I. Duchemin and X. Blase,

Phys. Rev. B 87, 245412 (2013). [4] X. Blase, C. Attaccalite, V. Olevano, Phys. Rev. B 83, 115103 (2011).

MM 40.7 Wed 12:15 TRE Ma

Charge transfer from first principles: self-consistent GW applied to donor-acceptor systems — ●FABIO CARUSO^{1,2}, VIKTOR ATALLA¹, ANGEL RUBIO^{1,3}, MATTHIAS SCHEFFLER¹, and PATRICK RINKE¹ — ¹Fritz Haber Institute, Berlin, Germany — ²University of Oxford, UK — ³Universidad del País Vasco, San Sebastián, Spain

Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, if the ionisation potential of one molecule erroneously ends up above the electron affinity of the other. An unphysical fractional electron transfer will then result in weakly interacting DAS [1]. GW calculations based on first-order perturbation theory (G_0W_0) correct the level alignment. However, the ground state is unaffected by the G_0W_0 approach, and the charge-transfer properties remain on the level of the initial DFT calculation [1]. We demonstrate that self-consistent GW (scGW) – based on the iterative solution of the Dyson's equation – provides an ideal framework for the description of charge transfer in DAS. The scGW level alignment is in agreement with experimental reference data. In addition ground- and excited-state properties are described at the same level of theory. As a result, the electron density in DAS is consistent with the level alignment between donor and acceptor, leading to a qualitatively correct description of charge-transfer properties.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, and M. Scheffler, Phys. Rev. B 88, 165122 (2013).

MM 40.8 Wed 12:30 TRE Ma

What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set — ●GIOVANNI BORCHI¹, NGOC LINH NGUYEN¹, ANDREA FERRETTI², ISMAILA DABO³, and NICOLA MARZARI¹ — ¹École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — ²Centro S3, CNR-NANO, Modena, IT — ³Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

In this talk we present the results of benchmark calculations of the structure and electronic-structure of all molecules in the g2 set, using different flavours for Koopmans' compliant (KC) functionals. Results are compared not only to LDA and PBE, but also to orbital-density dependent calculations with the Perdew-Zunger self-interaction correction.

Our results assess the accuracy of Koopmans' compliant functionals in improving semilocal functionals to predict electronic eigenvalues and in particular ionization energies, with an accuracy that for molecules seems to be comparable or superior to that of many-body (GW) approaches. We also highlight how the Koopmans' condition tends to preserve the potential energy surface of the underlying functional, with higher reliability than e.g. PBE in structural predictions, while also providing good estimates of atomization energies.

The talk will also provide a general introduction to the theory of Koopmans' compliant functionals and their implementation in existing electronic structure codes.

Ref. Dabo *et al.*, PRB 82, 115121 (2010), and Psik highlight (2012).

MM 40.9 Wed 12:45 TRE Ma

The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results — DANIEL LÜFTNER¹, SIVAN REFAELY-ABRAMSON², MICHAEL PACHLER¹, MICHAEL G. RAMSEY¹, LEEOR KRONIK², and ●PETER PUSCHNIG¹ — ¹Institut für Physik, Karl-Franzens-Universität Graz, Austria — ²Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Quinacridone is an organic molecule (C₂₀H₁₂N₂O₂) utilized in the formation of organic pigments. It has also been discussed for usage in organic electronics particularly due to its stability under ambient conditions and its tendency to form self-assembled supramolecular networks. Here, we report on its electronic structure, both, for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal polymorphs. We employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory as well as GW corrections within a many-body perturbation theory framework. A comparison of the theoretical results obtained with the different levels of theory and a subsequent comparison with experimental data from angle-resolved photoemission spectroscopy emphasize the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. Furthermore the comparison indicates that the results obtained with OT-RSH greatly improve those of standard DFT functionals and achieve an agreement with experiment at the level of GW calculations, thus making the OT-RSH an alternative to the computationally more expensive GW approach.

MM 40.10 Wed 13:00 TRE Ma

GW many-body perturbation theory for electron-phonon coupling calculations — ●CARINA FABER^{1,2}, PAUL BOULANGER¹, IVAN DUCHEMIN^{1,2}, and XAVIER BLASE¹ — ¹Institut Néel, CNRS, Grenoble, France — ²INAC, CEA, Grenoble, France

We study within many-body perturbation theory the electron-phonon coupling in organic systems, taking as paradigmatic examples the fullerene molecule and the pentacene crystal [1,2]. We show that the strength of the electron-phonon coupling potential is dramatically underestimated at the LDA level, while GW calculations offer an excellent agreement with experiments [1]. Further, combining GW calculations of the electronic band structure and of the electron-phonon coupling in crystalline pentacene, we show that the hole bands dispersion can be reconciled with photoemission experiments, by solving non-perturbatively (DMFT) the effect of electron-phonon coupling on the electronic self-energy [2]. We finally explore various approximations that may allow to combine the GW formalism with convenient linear response formalisms beyond the frozen-phonon techniques. Our calculations are performed with the Fiesta package, a Gaussian based GW and Bethe-Salpeter code allowing all-electron or pseudopotential calculations with various resolution of the identity techniques and without any plasmon pole approximation [3,4].

[1] C. Faber *et al.*, Phys. Rev. B 84, 155104 (2011) [2] S. Ciuchi *et al.*, Phys. Rev. Lett. 108, 256401 (2012) [3] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [4] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012).

MM 41: Computational Materials Modelling VI - Dislocations

Time: Wednesday 11:30–13:00

Location: IFW D

MM 41.1 Wed 11:30 IFW D

Dislocation mediated diffusion mechanisms of carbon in α -iron — ●GH.ALI NEMATOLLAHI, BLAZEJ GRABOWSKI, DIERK RAABE, and JÖRG NEUGEBAUER — Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany

Experimental observations have revealed that dislocations can provide "diffusion short circuits", i.e., impurities can use the distorted lattice around dislocations to diffuse faster than in the perfect bulk region. This phenomenon is usually referred to as pipe diffusion. These accelerated diffusion paths help to redistribute impurities faster, especially in heavily deformed materials that contain high dislocation densities. This has important consequences e.g. for carbon redistribution in severely deformed pearlite - a steel with the highest strength among nanostructured materials. In the present study, empirical potentials in conjunction with the nudged elastic band method are used to study carbon diffusion in the vicinity of edge, screw and mixed dislocation in bcc iron. Our results show that there are low carbon diffusion barriers of ~ 0.2 eV (vs. 0.8 eV in bulk) for all three dislocation types. For edge dislocations the results are not fully conclusive as it is technically difficult to stabilize such a dislocation due to the low Peierls barrier. For screw dislocations the low diffusion barrier is perpendicular to the dislocation line prohibiting pipe diffusion. Finally, for mixed dislocations, the low diffusion barrier is parallel with the dislocation line and is the only type that explains the experimentally proposed accelerated short circuit diffusion.

MM 41.2 Wed 11:45 IFW D

Effects of carbon interstitials on Fe dislocation core mobility using atomistic-continuum coupling — ●KARTHIKEYAN CHOCKALINGAM, REBECCA JANISCH, and ALEXANDER HARTMAIER — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, Bochum, Nordrhein-Westfalen 44801

Besides iron, carbon is the most significant alloying element in steel. It has been observed that carbon segregates to dislocation cores to form so-called Cottrell clouds. This is energetically favorable due to the low solubility of C in the iron matrix and the release of strain at the dislocation core. The carbon clouds pin the dislocations, resulting in an increase in yield strength. To better understand the influence of carbon on dislocation core mobility, its influence on edge and screw dislocation was investigated. We found that the relative increase in critical stress is higher for an edge dislocation than for a screw dislocation.

For this analysis we implemented an atomistic-continuum framework in which the dislocation core is modeled atomistically, and the material away from the dislocation core is described in a continuum-elasticity finite-element approach. Thus, the atomistic domain is restricted to a small region around the core, resulting in a significant reduction of the number of atoms required to model a dislocation. Initially we use an embedded atom method (EAM) type potential for the interatomic interactions, but the coupled framework is not limited to a particular choice of interaction and can also be used in combination with ab-initio methods.

MM 41.3 Wed 12:00 IFW D

Understanding H-embrittlement on the atomic scale: Multiscale modeling of homogenous dislocation nucleation — ●GERARD LEYSON, BLAZEJ GRABOWSKI, and JÖRG NEUGEBAUER — Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Hydrogen enhanced local plasticity (HELP) is one of the proposed mechanisms by which hydrogen induces embrittlement in metals. A promising methodology to explore the HELP mechanism is through nano-indentation experiments, wherein the effect of hydrogen on the pop-in load is precisely measured. Using the Ni-H system as a model system, an analytic model is developed to quantify the effect of hydrogen on the Homogenous Dislocation Nucleation (HDN) assumed to be responsible for the reduction of the pop-in load. The model takes atomistic inputs, such as hydrogen-hydrogen interaction and the effect of realistic dislocation cores, into account. The hydrogen binding energy and the local hydrogen concentration were calculated self-consistently. Unlike previous analyses, the model takes into account the complex nature of the dislocation field around the loops, as well as the discrete nature of the atomic lattice. In doing so, it addresses some short-

comings of previous models stemming from the continuum description of the dislocation line energy and the interaction of the dislocation with the external stress field. The onset of HDN as a function of bulk hydrogen concentration and temperature was quantified. Our results show that about 10-100 H atoms are sufficient to stabilize a dislocation loop in the presence of realistic shear stresses and allows for a quantitative description of the experimentally observed pop-in effects.

MM 41.4 Wed 12:15 IFW D

Metadislocation core structure in the ϵ -Al-Pd-Mn phases — BENJAMIN FRIGAN and ●HANS-RAINER TREBIN — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

In the past we have energy optimized the bulk structures of the ϵ -phases and the 16 Å decagonal phase of Al-Pd-Mn using density functional theory (DFT) and classical molecular dynamics. All phases consist of columns of pseudo-Mackay icosahedra (PMI) whose projections form tilings of hexagons, pentagons and nonagons in the ϵ -phases and several other tiles in the decagonal phase.

Most parts of the metadislocation cores in the ϵ -phases display the same cluster arrangements as in the bulk phases. Nevertheless, in small sections of the cores the usual cluster description fails. Recent microscopy images indicate that the central parts contain $1/\tau$ shorter PMI-PMI next-neighbor distances. The structure of these novel cluster intersections has been resolved with DFT calculations using the smallest possible approximant which contains such interpenetrating PMI clusters.

We present a full structure description of the metadislocation cores F_3 and F_5 . Embedded in bulk structures of ϵ -phases the cores have been relaxed using a combination of classical molecular dynamics and a Monte Carlo method where the chemical species were randomly flipped.

MM 41.5 Wed 12:30 IFW D

Dislocation – grain boundary interactions in aluminum: insights from atomistic simulations on bi-crystalline and nanocrystalline samples — ●JULIEN GUÉNOLE, ARUNA PRAKASH, and ERIK BITZEK — Department of Materials Science and Engineering, Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

The interactions between dislocations and grain boundaries (GB) are a dominating factor in the plasticity of nanocrystalline metals. Atomistic simulations have played a key role in improving our understanding of the atomic scale processes that govern dislocation-GB interactions. However, most studies so far have been performed on either quasi-2D bicrystal set-ups with straight dislocation lines or on unrealistic nanocrystalline samples generated by Voronoi tessellation. In both cases, the dislocations interact with planar GBs.

Here, we present results of controlled studies on dislocations interacting with GBs in model bi-crystalline samples as well as in more realistic nanocrystalline samples. The deposition process of curved dislocations is compared to the absorption of straight dislocations in a quasi-2D set-up. In addition, the stress-signature of the absorbed dislocation is analyzed. The results are compared with the absorption and pinning of dislocations at curved and planar GBs in nanocrystalline samples with controlled GB network topology. 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 41.6 Wed 12:45 IFW D

Atomistic Simulations of Dislocation-Interface Interactions in the γ/γ' Microstructure in Ni-based Superalloys — ●JUAN WANG, JULIEN GUÉNOLE, ARUNA PRAKASH, and ERIK BITZEK — Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Single crystalline Ni-base superalloys are key materials for turbine blades in modern gas turbines. The microstructure of these alloys consist of cubic γ' precipitates of Ni₃Al in the L1₂ crystal structure embedded in a γ -matrix of fcc Ni. The interaction of dislocations in the γ channels with the γ' precipitates is a main factor for the superior strength of these alloys even at high temperatures. The cutting of the dislocations from the γ channels into the precipitates is governed

by processes at the atomic scale. However, only few atomistic simulations of the dislocation behavior at the γ/γ' -interface have so far been performed. Here we report on a detailed study of screw and 60° dislocations interacting with a planar γ/γ' -interphase boundary in a quasi-two dimensional set-up. Static calculations as well as molecular dynamic calculations were performed to determine the critical penetration stress and to study the interaction of the channel dislocations

with the misfit dislocation network. In addition, the interaction of dislocations with a curved interphase boundary was studied in a fully 3D set-up modeling an experimental microstructure obtained by 3D Atom Probe Tomography. The results of the simulations are discussed in the framework of a multiscale modeling approach to study the mechanical behavior and stability of Ni-based superalloys.

MM 42: Electron Microscopy II - Advances in characterisation

Time: Wednesday 12:00–13:00

Location: IFW B

MM 42.1 Wed 12:00 IFW B

High-Energy Plasmons in MoS₂ and graphene heterostructures — ●MICHAEL MOHN¹, RALF HAMBACH¹, PHILIPP WACHSMUTH¹, GERD BENNER², and UTE KAISER¹ — ¹Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm, Germany — ²Carl Zeiss Microscopy GmbH, 74447 Oberkochen, Germany

We investigate high-energy plasmons using momentum-resolved electron energy-loss spectroscopy and ab-initio calculations for molybdenum disulfide (MoS₂) mono- and multilayers and MoS₂-graphene heterostructures.

Energy-loss spectra up to 50 eV have been obtained using a Zeiss Libra 200 based low-voltage transmission electron microscope (SALVE I [1]) with an in-column energy filter. The plasmon dispersion has been studied for momentum transfers along different crystallographic axes within the Brillouin zone. Ab-initio calculations have been performed with density functional theory (DFT) and linear-response time-dependent DFT using ABINIT and the dp-code [2,3]. By direct comparison of experimental spectra and ab-initio calculations, we address the following questions:

(i) How do high-energy plasmons in MoS₂ monolayers and multilayers behave for different momentum transfer? (ii) How do electron-energy loss spectra of MoS₂-graphene heterostructures differ from the spectra of the bare monolayers?

- [1] Kaiser et al., Ultramicroscopy 111, 1246 (2011)
- [2] Gonze et al., Comp. Mat. Sci. 25, 478 (2002)
- [3] Olevano, Reining, Sottile, <http://www.dp-code.org> (1998)

MM 42.2 Wed 12:15 IFW B

Feasibility study of using electron vortices for the measurement of electron magnetic circular dichroism (EMCD) — ●SEBASTIAN SCHNEIDER^{1,2}, DARIUS POHL¹, LUDWIG SCHULTZ^{1,2}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — ²TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

EMCD, which is the electron wave analogue of X-ray magnetic circular dichroism (XMCD), offers the possibility to study magnetic properties on the nanoscale in a transmission electron microscope (TEM). Recently discovered electron vortex beams, which carry an orbital angular momentum, are assumed to show comparable dichroic signals. This study is focused on the feasibility of this newly discovered method. Dichroic signals on the L₂ and L₃ edges of 3d transition metals are expected to be of the order of only 5%. In order to measure such small intensity changes in the electron energy loss (EEL) spectra, a proper microscope alignment, highly stable samples, and a high signal-to-noise-ratio of the EEL spectra are indispensable. Neglecting any of these preconditions will easily lead to artifacts showing a mime of a dichroic signal already in the raw data of the EELS spectra. Different types of magnetic samples are investigated and probed for the appearance of a dichroic signal thereby always paying highest attention to accurate measurements to avoid boosting any signals without physical relevance to EMCD. For this, thin ferromagnetic films of Fe, Fe₃C and Ni are prepared by sputtering and investigated with this novel method.

MM 42.3 Wed 12:30 IFW B

Probing atomic potentials on a sub-Angstrom scale by differential phase contrast — ●JOSEF ZWECK¹, SORIN LAZAR², BERT FREITAG², KNUT MÜLLER³, ANDREAS ROSENAUER³, FLORIAN KRAUSE³, MATTHIAS LOHR¹, BENEDIKT BAUER¹, ANDREAS PRITSCHET¹, and JOHANNES THALMAIR¹ — ¹Physics Faculty, University of Regensburg, FRG — ²FEI Company, Eindhoven, NL — ³Institute for Solid State Physics, University of Bremen, FRG

Differential phase contrast uses a position sensitive detector to monitor minute deflections of the electron beam in a scanning transmission microscope (STEM). With today's instruments, the electron beam can be focused into probe diameters of 80 pm, which is sufficiently small to move the probe within a unit cell of a crystal between atomic positions. The beam is influenced by the local Coulomb scattering potential of the atom. The scattering potential gradient across the electron beam diameter can in a first approximation be considered to be proportional to the local electric field caused by the nucleus and screened by the electron cloud.

Therefore, measuring the electron beam's deflection one probes a quantity related to the local field distribution. We present first results, obtained from a GaN crystal, and using a FEI Titan cubed, equipped with a high brightness gun, monochromator, an image Cs corrector and DCOR probe corrector. We can clearly show that the electron beam deflection is not radially symmetric around Ga and N atoms, which may lead to a technique capable to probe local binding structures and even electronic charge densities in sub-Angstrom resolution.

MM 42.4 Wed 12:45 IFW B

4D X-ray microscopy (XRM), In Situ imaging of practical volume samples — ●LARS-OLIVER KAUTSCHOR — Carl Zeiss Microscopy GmbH

In situ, 4D microscopy using X-ray microscopy is evolving as a valuable scientific technique. In order to develop this further it is important to develop the technique using realistic representative volumes in a wide range of materials. It is also important to evaluate the efficacy of the application against more traditional methods by employing correlative imaging. Conventional electron and optical microscopy techniques require the sample to be sectioned, polished or etched to expose the internal surfaces for imaging. However, such sample preparation techniques have traditionally prevented the observation of the same sample over time, under realistic three-dimensional geometries and in an environment representative of real-world operating conditions. X-ray microscopy (XRM) is a rapidly emerging technique that enables non-destructive evaluation of buried structures within hard to soft materials in 3D, requiring little to no sample preparation. Furthermore in situ and 4D quantification of microstructural evolution under controlled environment as a function of time, temperature, chemistry or stress can be performed repeatably on the same sample, using practical specimen sizes ranging from tens of microns to several cm diameter, with achievable spatial imaging resolution from submicron to 50 nm.

MM 43: Liquid and Amorphous Metals II - Mechanical properties

Time: Wednesday 11:45–13:00

Location: IFW A

MM 43.1 Wed 11:45 IFW A

FeCoSiBNbCu bulk metallic glass with large compressive deformability studied by time-resolved synchrotron X-ray diffraction — ●MIHAI STOICA^{1,2}, SERGIO SCUDINO¹, JOZEF BEDNARCIK³, IVAN KABAN^{1,4}, and JÜRGEN ECKERT^{1,4} — ¹IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, D-01069 Dresden, Germany — ²POLITEHNICA University of Timisoara, P-ta Victoriei 2, Timisoara, Romania — ³Deutsches Elektronen-Synchrotron (DESY), FS-PE Group, Notkestr. 85, D-22607 Hamburg, Germany — ⁴TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

By adding 0.5 at.% Cu to the strong but brittle $[(\text{Fe}_{0.5}\text{Co}_{0.5})_{0.75}\text{Si}_{0.05}\text{B}_{0.20}]_{96}\text{Nb}_4$ bulk metallic glass, fully amorphous rods with diameters up to 2 mm were obtained. The monolithic samples with 1 mm diameter revealed a fracture strain of 3.80 % and a maximum stress of 4143 MPa upon compression, together with a slight work-hardening behavior. An estimate of the temperature rise ΔT in the shear plane gives 1039 K, which is large enough to melt a layer of 120 nm. Mechanical tests performed in-situ under synchrotron radiation allowed the calculation of the strain tensor components, using the reciprocal-space data and analyzing the shift of the first (the main) and the second broad peak positions in the X-ray diffraction patterns. The results revealed that each atomic shell may have a different stiffness, which may explain the macroscopic compressive plastic deformation.

MM 43.2 Wed 12:00 IFW A

Diffusion, Structure and Crystallization in a HPT-deformed bulk metallic glass — ●JONAS BÜNZ¹, KOICHI TSUCHIYA², SERGIY DIVINSKY¹, and GERHARD WILDE¹ — ¹Institut für Materialphysik, WWU Münster, Germany — ²National Institute of Materials Science, Tsukuba, Japan

Metallic glasses show unique properties compared to their crystalline counterparts, but their applicability is limited by the lack of sufficient plasticity. Stress localization and the associated shear softening strongly weaken the structure, thus leading to the formation of shear bands. The structure of shear bands is still far from being understood. The HPT-technique allows the deformation of glasses with very high strains and thus leads to a rejuvenation of the structure and shear band densities which are obtainable with almost no other experimental technique. Thus, severely deformed glasses can act as a model system for integral testing methods such as calorimetry or diffraction analysis. Due to their extreme sensitiveness to the free volume localization, the diffusion measurements by the radiotracer technique can bring further insight into the structural modifications of shear bands with respect to the amorphous matrix as well as to the conditions of shearing during plastic straining. Here, the results of a combined study of diffusion process, crystallization behaviour and structure evolution in a HPT-deformed Zr-based bulk metallic glass are reported.

MM 43.3 Wed 12:15 IFW A

Mechanical behaviour of CuZr-based bulk metallic glasses and composites — ●BENJAMIN ESCHER^{1,2}, SIMON PAULY¹, IVAN KABAN^{1,2}, UTA KÜHN¹, and JÜRGEN ECKERT^{1,2} — ¹IFW Dresden, Institute for Complex Materials, P.O. Box 270116, 01171 Dresden, Germany — ²TU Dresden, Institute of Materials Science, 01062 Dresden, Germany

Compared to crystalline alloys, bulk metallic glasses (BMGs) exhibit yield strengths close to the theoretical limit. However, BMGs generally show a low or no plastic strain under either tensile or compressive stresses. This drawback has to be overcome for BMGs to be used as structural material.

The tolerance towards failure of CuZr-based BMGs can be significantly improved by the incorporation of structural heterogeneities such as crystals. The formation of such composites strongly depends on composition and cooling rate.

In the present work we investigated the mechanical properties of CuZr-based bulk metallic glasses and composites with different Al, Ag, Co and Sc additions. The effect of the elements on the thermal behaviour, the corresponding phase evolution and the resulting microstructure is correlated with the deformation behaviour.

It has been found, that the plasticity of the CuZr-X metallic glasses or composites can be significantly enhanced by the addition of proper quantities of the afore mentioned elements by changing the precipitating phase, its volume fraction and distribution.

MM 43.4 Wed 12:30 IFW A

Effect of micro-alloying on the properties of Pd- and Zr-based bulk metallic glasses — ●DAVIDE GRANATA, ERWIN FISCHER, and JÖRG F LÖFFLER — ETH Zürich, Zürich, Schweiz

For applications of bulk metallic glasses (BMGs) it is important to design new glass-forming alloys with improved properties. However, good glass-forming ability and improved mechanical properties, such as high fracture toughness and ductility, appear to be mutually exclusive. It has been shown recently that minor additions of suitable elements significantly alter the resulting properties of BMGs. In this micro-alloying approach slight compositional adjustments on the order of 0.1% generate drastic changes in critical casting thickness and mechanical characteristics. In this context we will discuss the role of fluxing-induced micro-alloying in the case of Pd-based BMGs. The knowledge gained will also be transferred to Zr-based BMGs, which are of greater interest for applications.

MM 43.5 Wed 12:45 IFW A

atomic structures and magnetic properties of FeB-based amorphous alloys — ●GUANGCUN SHAN^{1,2}, JILIANG ZHANG¹, and CHAN-HUNG SHEK¹ — ¹Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR — ²Max-Planck-Institut für Chemische Physik fester Stoffe

Several FeB-based amorphous alloys (Fe₈₀B₈Si₁₂, Fe₇₁B₁₇Si₁₂ and Fe₇₁B₁₇(Nb₄Y₄Zr₄)) with good mechanical properties and soft magnetic properties have recently been well developed by addition of solute atoms to tune the magnetic properties and glass forming ability (GFA). The atomic structures were revealed by state-of-the-art extended X-ray absorption fine structure spectroscopy (EXAFS) combining with ab initio molecular-dynamics (AIMD) computational techniques. Both AIMD computational results and the EXAFS spectra present clear evidence of a very different chemical and topological short-range order (SRO) around the Fe atom in all the studied samples. The experimental results of nanoindentation, XPS and thermal stability were in good agreement with the EXAFS results. Besides, the magnetic behaviors were discussed in view of the EXAFS results and atomic clusters of the glassy alloys.

MM 44: Festsitzung zum 50jährigen Bestehen der AG MM / Celebrating the 50th anniversary of the AG MM

The Metal- and Materials Division holds a honorary meeting to celebrate its 50th anniversary. The festive programme closes with the best poster prize presentation, which is awarded for the first time, and a reception.

Time: Wednesday 15:15–19:00

Location: BAR Schön

MM 44.1 Wed 15:15 BAR Schön
Opening remarks — ●JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

MM 44.2 Wed 15:20 BAR Schön
Topical Talk
Seeing the atoms in oxides, what is the use of it? — ●KNUT URBAN — Research Centre Juelich, 52425 Juelich, Germany

MM 44.3 Wed 15:50 BAR Schön
Topical Talk
From Phonons to Functionality — ●WINFRIED PETRY — TU München, München, Germany

MM 44.4 Wed 16:20 BAR Schön
Topical Talk

High Temperature Superconducting Materials and their Application for Levitation — ●LUDWIG SCHULTZ — IFW Dresden, Dresden, Germany

MM 44.5 Wed 16:50 BAR Schön
Topical Talk
The Division of Metal- and Materials Physics — ●MATHIAS GÖKEN — University Erlangen-Nürnberg, Erlangen, Germany

Best poster award

Empfang / Reception

MM 45: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V (O with HL/TT/MM)

Time: Wednesday 16:00–19:15

Location: TRE Ma

MM 45.1 Wed 16:00 TRE Ma
Topical Talk
Theory of nonlinear phononics for coherent light-control of solids — ●ANTOINE GEORGES^{1,2,3}, ALASKA SUBEDI², and ANDREA CAVALLERI⁴ — ¹College de France, Paris, France — ²Ecole Polytechnique - CPHT, Palaiseau, France — ³University of Geneva, DPMC, Switzerland — ⁴Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The use of light to control the structural and electronic properties of solids is an area of great current interest. We present a microscopic theory [arXiv:1311.0544] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations. Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman-active mode can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först et al. [Nature Physics 7, 854 (2011)] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini et al. [Rini et al. Nature 449, 72 (2007)]. We also predict a new non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.

MM 45.2 Wed 16:30 TRE Ma
DFT+Frontier Orbital U — ●EMINE KUCUKBENLI and NICOLA MARZARI — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Piecewise linearity of the total energy with respect to occupations is not only a fundamental property that should be obeyed by any exact energy functional, but also a starting point to improve approximate functionals that are used in practical applications.

DFT+U enforces piecewise linearity on the Hubbard manifold [1], and it has been shown to greatly improve the accuracy of density-functional theory for transition-metal complexes, thanks to its correction of self-interaction errors [2]. However, it still performs poorly in complexes where significant covalency is present, and intersite corrections (so-called DFT+U+V) have been introduced to improve these challenging cases [3].

Here, we revisit piecewise linearity within the DFT+U and DFT+U+V correction schemes, and explore a novel approach where self-interaction corrections are applied directly to the frontier orbitals. We test this approach on model transition metal complexes, where

highly accurate reference results can be established, and on small molecules with varying degrees of covalency.

References: [1] M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 35105 (2005). [2] H. J. Kulik, M. Cococcioni, D. A. Scherlis and N. Marzari, Phys. Rev. Lett. 97, 103001 (2006). [3] V. Leiria Campo Jr and M. Cococcioni, J. Phys. Cond. Matt. 22, 055602 (2010); H. J. Kulik and N. Marzari, J. Chem. Phys. 134, 094103 (2011).

MM 45.3 Wed 16:45 TRE Ma
Quasiparticle self-consistent GW method with spin-orbit coupling applied to Bi and HgTe — ●CHRISTOPH FRIEDRICH, IRENE AGUILERA, MARKUS BETZINGER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present an implementation of the quasiparticle self-consistent (QS) GW method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than being added *a posteriori*. The implementation is based on the FLAPW method. The SOC gives rise to spin off-diagonal blocks in the Green function G^{SOC} and the self-energy $\Sigma^{\text{SOC}} = iG^{\text{SOC}}W^{\text{SOC}}$. We applied the QSG^{SOC}W^{SOC} method to the semimetal Bi, which presents in experiment small electron and hole pockets and a tiny band gap (11-15 meV) at the L point, all of them largely overestimated by LDA (e.g., the gap is 86 meV). The QSG^{SOC}W^{SOC} approach predicts a value of the band gap of 8 meV and electron and hole pockets in very good agreement with experiment. The *a posteriori* treatment of the SOC (QSGW+SOC), on the other hand, yields an unphysical result for Bi, predicting it to be a topological insulator with a very large gap at L (260 meV) instead of a trivial semimetal. Similarly, for HgTe, QSGW+SOC reorders the bands in a wrong way and opens a gap at the Γ point in disagreement with experiment. In contrast, the QSG^{SOC}W^{SOC} approach yields a qualitatively and quantitatively correct description of the electronic band structure. We acknowledge support from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

MM 45.4 Wed 17:00 TRE Ma
Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the GW approximation — ●TIMO SCHENA, GUSTAV BIHLMAYER, CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

FeS₂ pyrite and marcasite have recently gained renewed interest as materials for photovoltaic applications, due to their large optical absorption and abundance. Therefore, a reliable description of the fundamen-

tal band gap of these compounds within first-principles calculations is desirable. However, common density functional theory (DFT) often suffers from an underestimation of band gaps. This calls for beyond-DFT methods, *e.g.*, the *GW* approximation, which is known to yield gaps in much better agreement with experiment. Although this is widely accepted for “simple” semiconductors, the situation is not well understood for more complicated cases, where the band edges differ in atomic and orbital character. In fact, we observe an uncommon band gap reduction in FeS₂ when applying single-shot *GW* on top of DFT, which might be problematic for photovoltaic applications [1]. In this work, we investigate the effects of the *GW* approximation on a couple of pyrite and marcasite compounds, employing the FLAPW code FLEUR and the *GW* code SPEX (www.flapw.de). In addition to single-shot *GW*, we also compare to the results of the recently implemented quasi-particle self-consistent *GW* approximation. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] T. Schena *et al.* Physical Review B (accepted 2013)

15 min. break

MM 45.5 Wed 17:30 TRE Ma

Probing d-band Quantum Well States in Palladium Nanofilms — ●SRIJAN KUMAR SAHA¹, SUJIT MANNA¹, MAREK PRZYBYLSKI^{1,2}, VALERI STEPANYUK¹, and JURGEN KIRSCHNER^{1,3} — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — ²Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — ³Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present the results of our new study which probes the d-bands quantum well (QW) states in Pd nanofilms grown on Cu(001) using first-principles density functional theory (DFT) calculations combined with scanning tunneling spectroscopy (STS) experiments. This study reveals that QW states occur in the overlayer films of Pd over a strikingly large film thickness (up to 17 monolayers) and in a large binding energy range (from 0.1 to 3.0 eV below Fermi level), thanks to its distinct and broad 4d-bands. The orbital characters of these states are unambiguously identified by our DFT calculations. Calculations also demonstrate oscillatory multilayer relaxations and d-derived quantum size oscillations in Pd films. The pseudomorphic growth, well-defined interface, and spatially resolved STS allows us to probe individual occupied QW states and extract the accurate dispersion of the (Δ_5 -like) d electronic band, as these states are laterally highly localized and give rise to distinct and sharp feature in the tunneling spectra.

MM 45.6 Wed 17:45 TRE Ma

Implementation and analysis of a plane wave and real space pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures — ●FRANK ZIRKELBACH, PIERRE-YVES PRODHOMME, JEROME JACKSON, and GABRIEL BESTER — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The implementation of the *large-scale atomic effective pseudopotential program* to solve the Schrödinger equation of an electronic system is discussed. *Atomic effective pseudopotentials* that are derived from screened local effective crystal potentials of self-consistent density functional theory (DFT) calculations are utilized, which ensure an accurate treatment at reduced computational costs. The capability of describing relevant electronic eigenstates of a quantum dot structure consisting of hundred thousand atoms at an atomistic *ab initio* level comparable to DFT is demonstrated. The possibility to represent the wavefunction and to evaluate parts of the Hamiltonian either in a plane wave or real space basis allows for a coherent analysis of various different approaches. In the fully real space treatment, linear scaling with respect to the system size is achieved. The convergence behavior of the different methods and utilized approximations is shown. Furthermore, an efficient spin-orbit treatment different to previously existing implementations within the pseudopotential formalism is outlined. The accuracy of the method is demonstrated via direct comparison to standard DFT codes.

MM 45.7 Wed 18:00 TRE Ma

Strong Parallelization of Real-Space DFT Calculations — ●ANDREA NOBILE^{1,2}, PAUL BAUMEISTER^{1,2}, DANIEL WORTMANN¹, and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Ger-

many — ²Jülich Supercomputing Center, Forschungszentrum Jülich, 52425 Jülich, Germany

The rapid change in modern supercomputing architectures poses a challenge to well established DFT codes. In particular, the increase in raw floating point power obtained through parallelism at different levels is not easily exploitable by using the traditional direct diagonalization methods. We will present our new real-space Projector Augmented Wave (PAW) implementation. The real-space representation of the wave functions, densities and potentials, enables the usage of very flexible boundary conditions and naturally adapts to massively parallel architectures. Parallelism can be exploited in the form of domain decomposition of the three dimensional grid, k-point sampling and bands. The kinetic energy operator, realized as a finite difference stencil, is localized. As a consequence the real-space representation of the Hamiltonian is sparse. This limits the amount of necessary communications and allows an application of the operator to a trial vector in order(N) operations. We will present results about the efficiency of the most numerical intensive parts of the code and we will compare the accuracy of the calculations for reference systems with other established DFT methods.

MM 45.8 Wed 18:15 TRE Ma

Rare Earth Metals in Density-Functional Theory — ●MARCO CASADEI¹, XINGUO REN², PATRICK RINKE¹, ANGEL RUBIO^{1,3}, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin — ²University of Technology, Hefei, China — ³NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

The presence of *f* electrons in the rare earths and their interaction with the *s* and *p* electrons give rise to several physical phenomena. One prominent example is the isostructural α - γ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the *f* electrons. We then addressed the question: *is the isostructural volume collapse in cerium unique?* By applying DFT, we studied lanthanum (La), praseodymium (Pr) and neodymium (Nd), which undergo several structural changes with pressure. We find that the transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that *f*-electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no *f*-electrons, and more than one stable solution in the fcc crystal for Pr and Nd, as found for Ce. Unlike in Ce, however, there is always one solution that is the most stable, thus no isostructural volume collapse emerges in agreement with experiments. [1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

MM 45.9 Wed 18:30 TRE Ma

Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors — ●WANG GAO and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV.

Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions play an increasingly larger role [2].

[1] G. X. Zhang, *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012).

[2] W. Gao and A. Tkatchenko, PRL **111**, 045501 (2013).

MM 45.10 Wed 18:45 TRE Ma

Scaling Laws for van der Waals Interactions in Nanos-

structured Materials — ●VIVEKANAND GOBRE and ALEXANDRE TKATCHENKO — Fritz Haber Institut der MPG, Berlin

Accurate description of van der Waals (vdW) interactions is crucial for precise prediction of structure and stability of complex materials. VdW forces originate from interactions between fluctuating multipoles in matter and play a significant role in the self-assembly of nanostructured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2] to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly.

[1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

MM 45.11 Wed 19:00 TRE Ma

2D nanopatterns of shape-persistent molecular polygons on HOPG — ●STEFAN-S. JESTER, NINA SCHÖNFELDER, EVA SIGMUND, and SIGURD HÖGER — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent organic molecules with flexible side chains self-assemble at the solution/solid interface to form 2D nanoarchitectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures. A key issue is how the shape and symmetry of the backbones and their alkyl chain substitution pattern determine the shape and symmetry of the adsorbate patterns. Recently we focused on molecular polygons (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides.[1] In my talk I will give insight into the relation between Archimedean surface patterns and supramolecular 2D adlayers. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

MM 46: Mitgliederversammlung des Fachverbands Metall- und Materialphysik

Time: Wednesday 19:00–20:00

Location: BAR 205

MM 47: Invited Talk (Hauptvortrag) Robinson

Time: Thursday 9:30–10:00

Location: BAR 205

Invited Talk MM 47.1 Thu 9:30 BAR 205
Coherent X-ray Diffraction Imaging of Excitations in Metal Nanoparticles — ●IAN ROBINSON — University College London, UK — Research Complex at Harwell, UK

The physical reason why nanoparticles differ in structure from the bulk is fundamentally crystallographic. As with all surfaces, the missing-neighbour unit cells, which become removed to create a surface, cause a structural response. In a metal this is an inward relaxation, detectable as crystal strain. Where two surfaces meet along the edge of a crystal, the effect is enhanced. Nanocrystals are in precisely the size range which is dominated by these surface and edge properties. This results in a pattern of strain which follow the crystallographic structure of the particle. Certain simple properties of nanoparticles

can be explained through these structural differences. Coherent X-ray Diffraction can be used to study these effects within the three dimensional structure of nanocrystals. A key experiment will be discussed that uses this method to study the redistribution of strains on the surface of a Au nanocrystal by adsorption of a chemical layer [1]. Ultrafast imaging with free-electron laser sources allows visualization of the strain patterns in vibrating crystals [2].

[1] Differential stress induced by thiol adsorption on faceted nanocrystals, Moyu Watari, Rachel McKendry, Manuel Voegtli, Gabriel Aeppli, Yeong-Ah Soh, Xiaowen Shi, Gang Xiong, Xiaojing Huang, Ross Harder and Ian Robinson, *Nature Materials* **10** 862-866 (2011) [2] Ultrafast three dimensional imaging of lattice dynamics in gold nanocrystals J. N. Clark et al *Science* **341** 56 (2013)

MM 48: Topical session: X-ray and neutron scattering in materials science I - Coherent X-ray Diffraction Imaging of Excitations in Metal Nanoparticles

Time: Thursday 10:15–11:30

Location: BAR 205

MM 48.1 Thu 10:15 BAR 205
Structural study of CuZr and Cu₅₀Zr₄₅Al₅ metallic glasses in relation to their GFA and mechanical properties — ●IVAN KABAN^{1,2}, PAL JOVARI³, BENJAMIN ESCHER^{1,2}, ADAM WEBB⁴, TOM REGIER⁴, BRIGITTE BEUNEU⁵, VALENTIN KOKOTIN⁶, NORBERT MATTERN², and JÜRGEN ECKERT^{1,2} — ¹TU Dresden, Institute of Materials Science, Germany — ²IFW Dresden, Institute for Complex Materials, Germany — ³Institute for Solid State Physics and Optics, Budapest, Hungary — ⁴Canadian Light Source, Saskatoon, Canada — ⁵Laboratoire Leon Brillouin, CEA-Saclay, France — ⁶ThyssenKrupp Steel Europe AG, Duisburg, Germany

In this work we investigate the atomic structure of CuZr and Cu₅₀Zr₄₅Al₅ metallic glasses in view of their glass-forming ability and mechanical properties. Using a combination of the state-of-the-art experimental techniques (synchrotron X-ray diffraction and absorption spectroscopy and neutron diffraction), reverse Monte-Carlo simulation and Molecular Dynamics modelling we have obtained partial pair distribution functions, coordination numbers and bond lengths for the glasses studied. Remarkable differences are found for the total as well as for the partial pair distributions in the CuZr and Cu₅₀Zr₄₅Al₅ metallic glasses, especially for the Cu-Cu and Zr-Zr pairs at the sec-

ond and higher coordination shells, suggesting important role of the medium-range order in the glass formation and in the mechanical behaviour.

MM 48.2 Thu 10:30 BAR 205

Static atomic displacements of Fe-27 at.% Pt in the Invar regime — ●CÉDRIC SAX and BERND SCHÖNFELD — LMPT, Department of Materials, ETH Zurich

X-ray diffuse scattering from a single crystalline Fe-27.1 at.% Pt Invar alloy was measured at room temperature and close to the Curie temperature. The sample was set up in a short-range ordered state by quenching from 1120 K. As expected due to the nearby located L₁₂ ordered structure, diffuse maxima are seen close to the X position. Separation of the diffuse scattering into short-range order scattering and displacement scattering was performed by the method of Georgopoulos and Cohen. The short-range order parameters remain nearly unchanged for both measurements and yield effective pair interaction parameters that properly reproduce the order-disorder transition temperature. On the other side, differences are observed in the species-dependent static atomic displacements of the first two coordination shells for both measurements. This change close to the Curie temper-

ature is compared with literature data in Ni-Fe where two measurement temperatures were chosen well below the Curie temperature.

MM 48.3 Thu 10:45 BAR 205

Hydrogen desorption pathway of Mg(BH₄)₂ probed by in-situ X-ray Raman scattering — ●SIMON KUJAWSKI¹, CHRISTIAN STERNEMANN¹, ARNDT REMHOF², CHRISTOPH SAHLE³, YIGANG YAN², NICHOLAS STADIE², KOLJA MENDE¹, ALI AL ZEIN⁴, and METIN TOLAN¹ — ¹Fakultät Physik/Dortmund Electron Accelerator, Technische Universität Dortmund, 44221 Dortmund, Germany — ²EMPA, Swiss Federal Laboratories for Materials Science and Technology, Hydrogen & Energy, 8600 Dübendorf, Switzerland — ³Department of Physics, University of Helsinki, FI-00014, Helsinki, Finland — ⁴European Synchrotron Radiation Facility, F-38043 Grenoble Cedex 9, France

With a hydrogen density of 14.9 wt% the complex hydride Mg(BH₄)₂ is considered as a solid-state hydrogen storage material. Identifying the amorphous boron-containing species during the desorption process provides essential information about the decomposition pathway of Mg(BH₄)₂. Unlike diffraction, X-ray Raman scattering allows investigating the local atomic and electronic structure and hence quantitatively estimating the amounts of different amorphous constituents. By modelling the X-ray Raman spectra from the possible constituents we unveiled the reaction pathway and determined the role of boron within.

MM 48.4 Thu 11:00 BAR 205

Hydrogen absorption in Mg-Ti multilayers studied by neutron reflectometry — ●MAXIMILIAN SKODA¹, CHRISTIAN KINANE¹, RAYMOND FAN², SEAN LANGRIDGE¹, WILLIAM DAVID¹, ANDREA BALDI⁵, BERNARD DAM³, HERMAN SCHREUDERS³, and RONALD GRIESSEN⁴ — ¹ISIS, STFC, Harwell, UK — ²Diamond Light Source, Harwell, UK — ³TU Delft, Delft, The Netherlands — ⁴Department of Physics and Astronomy, VU Amsterdam, The Netherlands — ⁵Stanford University, Stanford, USA

Mg-Ti thin film alloys have large H-storage capacities, fast kinetics of hydrogen absorption and desorption and are structurally stable. These qualities stem from a short-range ordered distribution of the Mg and

Ti atoms. In order to study the influence of short-range order on the hydrogen sorption properties of Mg-Ti systems, we artificially engineered chemical segregation by depositing a Ti/Mg multilayer with 10 repetitions of Ti(2 nm)/Mg(4.4 nm). On exposure to H₂ a two-step hydrogenation process occurs with the Ti layers forming the hydride before Mg. In-situ, time resolved Neutron Reflectometry (NR) allows an accurate determination of the out-of-plane expansion associated with each hydrogenation step. The volume expansion expected for the hydrogenation of both Ti and Mg is transferred completely in the vertical direction, indicating that large plastic deformations have to occur upon hydrogen absorption. Owing to the large negative neutron scattering length of hydrogen, NR proves to be an excellent technique for the in-situ characterization of the hydrogen absorption properties of thin films.

MM 48.5 Thu 11:15 BAR 205

Electrode Lithiation in Lithium-Ion Batteries Investigated by In-Operando Neutron Reflectometry — BUJAR JERLIU¹, ERWIN HÜGER¹, BEATRIX-KAMELIA SEIDLHOFER², ROLAND STEITZ², and ●HARALD SCHMIDT¹ — ¹Clausthal University of Technology — ²Helmholtz-Zentrum Berlin

Lithium-ion batteries are widely developed and used as rechargeable power sources for portable electronic devices and will be essential in the field of automotive transportation. One of their major advantages is their low weight, and therefore the high energy density available. Kinetic processes and interface phenomena at electrodes during charging and discharging cycles play a key role for optimization of these batteries (e.g. for charging times and power density). As negative electrode material, amorphous silicon has become a promising candidate for future Li-ion battery applications due to its high theoretical specific capacity of about 4 Ah/g.

We present in-operando neutron reflectometry experiments on the lithiation of amorphous silicon electrodes during galvanostatic charging or during cyclic voltammetry. Such studies allow to monitor the modification of Li content and the corresponding volume expansion/contraction of the electrode during lithiation on the nanometer scale. Possible lithiation mechanisms are discussed.

B. Jerliu et al. Phys. Chem. Chem. Phys., 15 (2013) 7777.

MM 49: Computational Materials Modelling VII - Grain boundaries & Interfaces

Time: Thursday 10:15–11:45

Location: IFW D

MM 49.1 Thu 10:15 IFW D

Theoretical study of hydrogen trapping and diffusion at grain boundaries in nickel — ●DAVIDE DI STEFANO¹, MATOUS MROVEC^{1,2}, and CHRISTIAN ELSAESSER^{1,2} — ¹Fraunhofer IWM, Freiburg, Germany — ²Karlsruhe Institute of Technology, Karlsruhe, Germany

A correct description of hydrogen diffusion in metals is a prerequisite for understanding the phenomenon of hydrogen embrittlement. It is known that H mobility in metals is strongly affected by lattice defects such as vacancies, dislocations or grain boundaries. It is however rather difficult to investigate local diffusion and trapping of H at these nanoscale defects by experimental means.

In this theoretical study, we explore the interaction of H with several grain boundaries (GBs) in Ni at the atomic scale using first principles calculations based on density functional theory (DFT). Our results are that GBs with open structural units act as trapping sites for H and provide also easy diffusion pathways for H. In contrast, GBs with close-packed structures similar to that of bulk fcc Ni do not trap H but act instead as barriers for H. In order to obtain information about H diffusion on long time and length scales, we developed a kinetic Monte Carlo model that can utilize the DFT results to calculate effective diffusion coefficients of polycrystalline microstructure.

MM 49.2 Thu 10:30 IFW D

Ab-initio study of hydrogen trapping by kappa-carbides in an austenitic Fe matrix — ●POULUMI DEY¹, ROMAN NAZAROV², TILMANN HICKEL¹, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — ²Lawrence Livermore National Laboratory 7000 East Avenue, Livermore, CA 94550

Experimental studies demonstrated that fine dispersed precipitates of carbides increase the tensile strength of steels and may act as deep

trapping sites for hydrogen. In this regard, homogeneously distributed nano-sized kappa-carbides (Fe,Mn)3AlC, have been found to play an analogous role in a new class of high strength Fe-Mn-Al-C steels. However, much less is known about the efficiency of these carbides in trapping hydrogen in these steels. We thus perform a quantitative analysis of hydrogen solution enthalpies within kappa-carbide precipitates employing density functional theory (DFT). While the solubility of hydrogen is low in perfect kappa-carbide, the presence of hydrogen makes the formation of vacancies energetically favourable, which in turn act as effective trapping sites for hydrogen. Further, motivated by the experimental investigations, we investigate the trapping of hydrogen at the interface between kappa-carbide and the austenitic matrix. Our results show that the interface is a potential trapping site for hydrogen and also a nucleation point for subsequent fracture in the material.

MM 49.3 Thu 10:45 IFW D

Ab-initio prediction of the critical thickness of a precipitate in molybdenum — ●SANKARI SAMPATH and REBECCA JANISCH — ICAMS, RUB, Bochum, Germany

The precipitation of new phases in a host metal or metallic alloy has a strong influence on the mechanical properties of the material. This precipitation leads to the formation of an interface that can be coherent, semi-coherent or incoherent with the host material. The calculation of coherent interface energies based on atomistic models is well established, but semi-coherent interfaces still present a challenge. Current approaches usually combine ab-initio data and continuum elasticity methods, while we now present a model for a semi-coherent interface completely based on ab-initio density functional theory calculations.

Our example is a metastable Mo-C phase, the body-centered tetragonal structure, which exists as a semi-coherent precipitate in body-centered cubic molybdenum. For the coherent interface, a standard supercell approach is used. The energy of the semi-coherent interface

is calculated taking into account different contributions from the elastic strain energy stored in the precipitate, the misfit energy due to the misfit dislocation, and the chemical energy due to the bonding at the interface. By comparing the energy of a coherent with that of a semi-coherent precipitate as a function of thickness, we predict a critical thickness of the precipitate before it becomes semi-coherent that agrees well with the experimental observation.

MM 49.4 Thu 11:00 IFW D

Hot or cold: A guide on how to determine an optimal simulation temperature in the Potts model for normal grain growth — ●DANA ZÖLLNER — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The simulation temperature in the Monte Carlo Potts model of grain growth is not correlated to any real experimental temperature and has originally been introduced into the simulation purely to activate thermal fluctuations that roughen the grain boundaries and prevent an unphysical lattice effect - namely the pinning of grain boundaries and their junctions to the underlying lattice.

In the present work it is shown that in the Monte Carlo Potts model there is for a given implementation of the simulation algorithm and a given set of lattice parameters a one-to-one correspondence between the simulation parameters γ and m representing the specific grain boundary energy and mobility in the simulation algorithm and the phenomenological parameters in the equation of motion only for one certain simulation temperature, T_{opt} . In particular, it is discovered that only the use of T_{opt} reproduces the curvature driven kinetics of normal grain growth, e.g., the von Neumann-Mullins-relation, correctly.

MM 49.5 Thu 11:15 IFW D

Atomistic simulation of a severe plastic deformation-induced "high-energy" state of grain boundaries — ●LISA NEIER¹, SERGIY DIVINSKI¹, ANANTHA PADMANABHAN², and GERHARD WILDE¹ — ¹Institut für Materialphysik, Westfälische-Wilhelms-Universität, 48149 Münster — ²University of Hyderabad, India

A comparison of microstructures and properties in materials subjected to the later stages of severe plastic deformation 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 and choosing oblate spheroids of a few atomic diameters size as the basic units of sliding. Atomistic simulations of these special GBs are performed. The coupling of grain boundary motion in normal direction to a shear deformation parallel to the grain boundary plane is investigated for these special grain boundaries in comparison to those of different relaxed high angle grain boundaries. Furthermore thermal equilibrium fluctuations of the grain boundaries during the MD simulations are used to calculate the grain boundary stiffness and analyze the influence of grain boundary structure and shear localization on the fluctuation spectrum.

MM 49.6 Thu 11:30 IFW D

Driving force and temperature dependence of grain boundary motion — ●CHRISTIAN BRANDL¹, DANNY PEREZ², TIMOTHY C. GERMANN², and OLIVER KRAFT¹ — ¹Karlsruhe Institute of Technology, Institute of Applied Materials, Karlsruhe, Germany — ²Los Alamos National Laboratory, Theoretical Division, Los Alamos, USA

The motion of interfaces - in particular grain boundaries (GBs) - is a fundamental mechanism of microstructure formation at high temperature and long time scales (annealing, coarsening). Moreover GB motion is also shown to be a deformation mechanism occurring at high stresses and relative low temperatures as in deformation studies of nanocrystalline metals and shock loading. Using MD simulations and transition search methods (string method), we report on the interface motion of an asymmetric GB in Cu to elucidate the role of atomistic structure (morphology) and velocity-driving force relation (mobility) as function of temperature. We show that the GB velocity as a function of temperature and driving-force shows distinct regimes of dynamics regimes ranging from pinning-depinning transition at low temperature, through rare-event dynamics of critical kink-pair disconnection nucleation along intrinsic GB dislocations to approximate temperature independent GB velocities. We will discuss the observation in the context of necessary ingredients for a mesoscale model of interface motion, which incorporates the atomic scale interface structure and the different regimes of driving-force and temperature.

MM 50: Mechanical properties III - Evolution & deformation of microstructure

Time: Thursday 10:15–12:00

Location: IFW B

MM 50.1 Thu 10:15 IFW B

Liquid Ga penetration into ultra-fine grained Al — ●MEHRNOOSH NADERI, SERGIY DIVINSKI, and GERHARD WILDE — Institute of Material physics, Münster, Germany

Under certain conditions, liquid metal can rapidly penetrate into a solid, typically along grain boundaries the phenomenon known as liquid metal embrittlement. One of the most spectacular examples of such phenomena is the gallium penetration into an aluminum grain boundary network. Most studies in this field relate the liquid penetration process to mechanical properties of the grain boundaries. In this work the penetration behavior of liquid Ga in ultrafine grained Al produced by high pressure torsion (HPT) was investigated by dilatometry. Penetration of liquid Ga induces an unexpected, two-stage evolution of free volume in ultra-fine grained Al. The developments of the grain boundary decoration by liquid Ga and the surface evolution have been examined by scanning electron microscopy and atomic force microscopy. The abnormal length change behavior is discussed in terms of underlying mechanisms that control the Ga penetration.

MM 50.2 Thu 10:30 IFW B

Viscoplastic properties of copper with ultrafine grain structure after high-pressure torsion — ●JÖRN LEUTHOLD, MATTHIAS WEGNER, MARTIN PETERLECHNER, SERGIY V. DIVINSKI, and GERHARD WILDE — Institute of Materials Physics, University of Muenster, 48149 Muenster, Germany

Metals processed by severe plastic deformation possess a high density of stored energy in the form of vacancies, dislocations, twins, high- and low-angle grain boundaries. As a consequence of the grain refinement towards the sub-micrometer range, the structure and thermal evolution

of grain boundaries as well as the interactions of the internal interfaces with defects in the grain interior become decisive factors for thermal stability, kinetic and plastic properties of the material. Even at low homologous temperatures, the viscoplastic flow can significantly contribute to the deformation mode when a mechanical stress is applied. In this study, 99.99% pure copper was processed by High Pressure Torsion (HPT) and investigated via nanoindentation. In addition to the determination of hardness maps, the viscoplastic properties were analyzed using long dwell times. Furthermore, uniaxial tensile tests were performed to determine the strain rate sensitivity in load jump tests. In combination with electron back scatter diffraction, the grain size and misorientation distribution and texture were analyzed in the as-deformed state and after additional tensile elongation at temperatures in the range from 293 K to 423 K. The results are discussed with respect to dislocation-mediated and grain boundary dominated mechanisms of plasticity.

MM 50.3 Thu 10:45 IFW B

Temperature-dependent shear behaviour of different grain boundaries in aluminium: An MD and metadynamics study — ●XUEYONG PANG and REBECCA JANISCH — ICAMS, Bochum, Germany

We investigate the temperature-dependent mechanical shear behaviour of different tilt and twist grain boundaries in aluminium employing molecular dynamics and metadynamics simulation methods with embedded-atom method type potentials. The goal is to relate the mechanical properties of interfaces to the features of the grain boundaries gamma- respectively free energy surface, and thus to the grain boundary structure and misorientation. In the molecular dynamics simulations two different kinds of deformation modes were used to see the

influence on the shear stress and the sliding mechanisms along different sliding directions, e.g. an easy-sliding and a general direction. Both molecular dynamics and metadynamics simulations were carried out at different temperatures to see the variation in energy barriers and shear strength as a function of temperature. The relation between structure and the obtained properties will be discussed in the presentation.

MM 50.4 Thu 11:00 IFW B

Room temperature grain growth in polymer-supported Cu and Au films during fatigue loading — ●OLEKSANDR GLUSHKO and MEGAN CORDILL — Erich Schmid Institute, Jahnstr 12, 8700 Leoben, Austria

In this contribution a systematic investigation of microstructural changes in polymer-supported Cu and Au films under tensile fatigue loading conditions is presented. Fatigue tests were performed under total strain control and electrical resistance of the films was measured in-situ during the test. To capture the changes in the grain structure due to fatigue the EBSD and FIB ion channeling techniques were applied to the same areas of the films once before and once after cyclic mechanical test. Using this approach significant grain coarsening was observed in e-beam evaporated 500 nm thick Cu and Au films on polyimide. The grain coarsening effect is also manifested by the decrease of film resistance during first 500-1500 cycles. Under certain conditions the grain coarsening in gold films leads to total recrystallization and grain sizes are increased by 400% already after 1000 cycles. The role of grain coarsening in initiation and propagation of fatigue damage is also discussed.

MM 50.5 Thu 11:15 IFW B

Mechanical alloying of Cu50Ta50 produced by high pressure torsion — ●NAZAR IBRAHIM, MARTIN PETERLECHNER, SERGIY DIVINSKI, and GERHARD WILDE — Institute of Materials Physics, Westfälische Wilhelms-University Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Mechanical alloying (MA) is generally considered as a solid-state powder processing technique, which involves repeated cold welding, fracturing and re-welding of powder particles in a high-energy ball mill. Recently, high pressure torsion (HPT) has been considered as a new MA method and was used for the fabrication of advanced materials with unique properties. In this work, HPT-induced mechanical alloying has been studied in the case of the immiscible Cu-Ta system. Cu and Ta foils with a thickness of 0.025 mm and a diameter of 10 mm were assembled alternately and subjected to HPT processing under an applied pressure of 4 GPa for 10, 30, 50, 100 and 150 turns at a rotational speed of 1.5 rpm. The phase constitution and microstructures were examined by X-ray diffraction, transmission and scanning electron microscopy. Additionally, the samples were characterized via microhardness measurements. It was shown that the HPT processing for 150 turns allows to completely mix Cu and Ta.

MM 50.6 Thu 11:30 IFW B

High-strength titanium-based materials processed by se-

lective laser melting — ●HOYAR ATTAR^{1,2}, MARIANA CALIN², LAI CHANG ZHANG¹, and JÜRGEN ECKERT^{2,3} — ¹Edith Cowan University, Perth, WA 6027, Australia — ²IFW Dresden, Institute for Complex Materials, P.O. Box 270116, D-01171 Dresden, Germany — ³TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

Titanium and its alloys are widely used in biomedical industries. Improvement of their mechanical properties plays an important role in enhancing the biomechanical compatibility of Ti-based implants, leading to increase their longevity in the human system. The traditional processing technologies utilized for manufacturing medical devices are usually highly time and material consuming processing steps. Selective laser melting (SLM) is providing the ideal platform for producing components with almost no geometric constraints and is economically feasible down to a batch size of one. In the present work, optimal manipulation of SLM parameters were used to produce high strength commercially pure titanium (CP-Ti) and Ti-TiB composites with superior properties than those of conventionally processed. Results showed that mechanical properties of SLM-processed CP-Ti have been significantly increased compared to those of traditionally manufactured. The noticeable improvement of mechanical properties of SLM-processed CP-Ti is result of ultrafine martensitic grains formed during the SLM process. Moreover, micro-hardness and compressive strengths of the CP-Ti were increased greatly when it was reinforced with TiB particles.

MM 50.7 Thu 11:45 IFW B

Influence of pressure during high pressure torsion of NiAl — ●CHRISTINE TRÄNKNER¹, ROBERT CHULIST², WERNER SKROTZKI¹, BENOÎT BEAUSIR³, THOMAS LIPPMANN⁴, JELENA HORKY⁵, and MICHAEL ZEHETBAUER⁵ — ¹Institut für Strukturphysik, Technische Universität Dresden, Dresden, Germany — ²Institut Metallurgii i Inzynierii Materialowej, Polskiej Akademii Nauk, Kraków, Poland — ³Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux, Université de Lorraine, Metz, France — ⁴Institut für Werkstofforschung, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ⁵Fakultät für Physik, Universität Wien, Wien, Austria

NiAl is an intermetallic compound with a brittle-to-ductile-transition temperature at about 300°C and ambient pressure. As shown in [1], fracture stress and fracture strain are increased under high pressure. Therefore, deformation at low temperatures is only possible at high pressures, as for instance used in high pressure torsion (HPT). In order to study the influence of pressure on texture evolution and microstructure formation, small discs of polycrystalline NiAl were deformed by HPT at temperatures ranging from room temperature to 500°C and pressures from 2 to 8 GPa. For low temperatures higher pressures lead to less cracking and slipping. Regarding texture, pressure mainly influences the intensities of the texture components. Grain size also changes with pressure. For deformation at 500°C, the grains in the 2 GPa sample are twice as large as in the material deformed at 8 GPa. The results will be discussed with regard to dynamic recrystallization.

[1] R. Margevicius et al., *Met. Mater. Trans. A* 25, 1994, 1457-1470.

MM 51: Liquid and Amorphous Metals III - Electronic properties of amorphous alloys

Time: Thursday 10:15–11:15

Location: IFW A

MM 51.1 Thu 10:15 IFW A

How structures form and properties emerge — ●PETER HÄUSSLER — Chemnitz University of Technology, Physics Institute, 09107 Chemnitz, Germany

The formation of crystals and the accompanied emergence of their physical properties are far from being understood. Quantum chemistry, statistical physics, as well as thermodynamics all play an indispensable role. But, each of them is unable to solve the problem alone. The formation of structure cannot be explained by interacting individual atoms alone, instead, their cooperative actions should properly be accounted too. Cooperatively acting species would reduce the tremendous number of parameters to a manageable level. In this contribution we report on global subsystems and their interaction. Under the given external constraints they form global resonances by self-organizing mutually their internal features, causing global anti-bonding as well as bonding states at different energies. Accordingly, by occupying the latter, both, the decrease of the total energy and

the creation of entropy become maximal. Pseudo-gaps arise at the Fermi energy and by this, major structural features are influenced. Electronic transport anomalies, the thermal stability, as well as many others emerging physical quantities are strongly influenced.

Our description follows the formal language of thermodynamics by an extended version (General Dynamics) applied to the global subsystems and introduces momentum as well as angular momentum, both included in quantum chemistry and statistical physics, but not in classical thermodynamics, so is able to form a bridge between them.

MM 51.2 Thu 10:30 IFW A

What do electron energy loss spectra of binary amorphous Al-TM alloys tell us? — ●MARTIN STIEHLER, SYED SAJID ALI GILLANI, PIERRE PUDWELL, HANS WEBER, and PETER HÄUSSLER — Technische Universität Chemnitz, D-09107 Chemnitz

Some time ago (*J. Phys. Chem. Sol.* **68** (2007) 1244) we reported on an intriguing systematic feature in the electron energy loss spectra of

binary *amorphous* (*a*) Al alloys with transition metals (TM) from the fourth period of the periodic table (3d-TM). If interpreted as caused by the excitation of volume plasmons the 3d-TM would have to be counted with a constant valency of 5 e/a irrespective of the particular 3d-TM and irrespective of their concentration in the alloy. In contrary to amorphous alloys without d-states at the Fermi edge this valency would not coincide with the “usual” valency used in calculating, for example, the Fermi-sphere diameter.

In our talk data on *a*-Al-(Ca,Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Y,Pd,Ce) is presented, showing that the aforementioned systematics can also be observed in systems with 4d- and 5d-TM. One possible explanation is based on the influence of inter-/intra-band transitions due to the d-states of the TM. For further insight we compare our results with literature data on systems with non-transition metals like Al-(Mg,Zn) in the *crystalline* state and with *amorphous* Ga-Mn alloys. The latter is to clarify the role of Al in the systems.

MM 51.3 Thu 10:45 IFW A

Amorphous Al-Pd Alloys – Structure and electronic properties — ●PIERRE PUDWELL, MARTIN STIEHLER, and PETER HÄUSSLER — Technische Universität Chemnitz, 09107 Chemnitz

The electronic influence on the formation of the static structure in condensed matter is known since decades. Furthermore, it is also known that not only the latter *subsystem* is able to adjust, but the *electronic subsystem* itself is also variable. Amorphous alloys were found to be perfectly suited to explore this *mutual* relationship which is based on an internal exchange of momentum between the two mentioned subsystems, in detail. Both subsystems try to come into *resonance* to each other. During the last years we reported on a particular variability of the electronic subsystem in Al-3d-TM alloys (TM: Sc, . . . , Cu) by *hybridization effects* between Al-3p- and TM-3d-states. In order to test whether such a *hybridization-enhanced resonance* is also effective in other systems, we are about to extend our investigations to systems with 4d- and 5d-TM.

In our contribution we show data on Al-Pd alloys as representative

for a system with 4d-TM. Thin films of the material with thicknesses around 50 nm were deposited in high-vacuum at cryogenic temperatures. The electrical resistivity was measured during annealing to several hundred K, the static atomic structure after annealing to 350K. By comparing the diameter of the strongest diffraction ring with the diameter of the Fermi-sphere, stabilizing resonances based upon different mechanisms, leading to several concentration regions with different structural and electronic behaviour, were identified.

MM 51.4 Thu 11:00 IFW A

Magnetic-Nonmagnetic Transition Observed by Disorder-Order Transition in Quasicrystalline AlPdFe Thin Films by means of Magnetotransport Properties — ●JOSE BARZOLA-QUIQUIA^{1,2}, MARTIN STIEHLE², and PETER HÄUSSLER² — ¹Abteilung Supraleitung und Magnetismus, Institut für Experimentelle Physik II, Universität Leipzig, Linnestr. 5, D-04103, Germany — ²Abteilung Physik Dünner Schichten, Institut für Physik, Technische Universität Chemnitz, D-09107, Germany

We report measurement results of the electrical resistivity, magnetoresistance and Hall effect of Al₇₀Pd₂₀Fe₁₀ alloy in amorphous and quasicrystalline phases. The measurements were performed in a temperature range of 1.2 to 300 K, applying fields of ±8 T. An anomalous contribution to the Hall effect, induced by the magnetic order is observed only in the amorphous phase, after the transformation to the ordered quasicrystalline phase, this anomalous contribution disappears. Atomic structure information obtained by transmission electron spectroscopy reveals that the local icosahedral order is already present in the amorphous phase and is improved by the transition to the quasicrystalline phase. SQUID magnetometry measurements verify the magnetic properties of the amorphous phase and confirm the parameters obtained from the resistance measurements. The experimental results can be understood in the frame of electronic stabilized systems, where hybridization effects of Al-*s, p* with Fe-*d* electrons, play an important role.

MM 52: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI (O with HL/TT/MM)

Time: Thursday 10:30–13:15

Location: TRE Ma

Topical Talk

MM 52.1 Thu 10:30 TRE Ma

Localization at the edge of 2D topological insulator by Kondo impurities — ●BORIS ALTSHULER¹, IGOR ALEINER¹, and VLADIMIR YUDSON² — ¹Physics Department, Columbia University, New York, NY 10027, USA — ²Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow 142190, Russia

Recent interest to the topological insulators [1] is inspired by the fact that their boundaries host gapless electronic excitations, which are extended and make the system conductive even in the presence of a potential disorder. 1D edge of a 2D topological insulator is predicted to have perfect conductance ($2e^2/h$): right and left moving electrons carry opposite spins and potential disorder cannot flip spins and thus causes neither back-scattering nor the usual 1D localization.

What if there are localized spins coupled to the edge electrons? It turns out that the conductivity is still perfect provided that this coupling conserves the z-projection of the total spin of the impurities and electrons. Magnetic anisotropy violates this conservation and causes the backscattering even at $T=0$, i.e. an arbitrary small density of the spins with arbitrary weak anisotropy of the coupling leads to Anderson localization of the edge states in long enough samples [3]. The conclusion follows from the mapping of the electron-spin coupling to the well-studied problem [2] of disordered Luttinger liquid.

1. M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2. T.Giamarchi and H.J.Schulz, Phys. Rev. B 37, 325 (1988).
3. B.L.Altshuler, I.L.Aleiner, V.I. Yudson Phys. Rev. Lett 111, 086401 (2013)

MM 52.2 Thu 11:00 TRE Ma

Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures — ●STEFAN WIPPERMANN¹, MARTON VÖRÖS², DARIO ROCCA³, ADAM GALI⁴, GERGELY ZIMANYI², and GIULIA GALLI² — ¹Max-Planck-Institute for Iron Research, Düsseldorf — ²University of California, Davis — ³Universite de Lorraine, Nancy

— ⁴Budapest University of Technology and Economics

Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si. However, the increased efficiency is observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum.

We present density functional and many body perturbation theory calculations of the electronic, optical, and impact ionization properties of Si and Ge nanoparticles (NPs) with core structures based on high-pressure bulk Si and Ge phases. Si and Ge particles with a BC8 or ST12 core structure exhibit significantly lower optical gaps and multiple exciton generation (MEG) thresholds, and an order of magnitude higher MEG rate than diamondlike ones of the same size (1).

- (1) S. Wippermann et al., Phys. Rev. Lett. 110, 046804 (2013)

MM 52.3 Thu 11:15 TRE Ma

Advanced time-evolution method for optical absorption spectra calculations — ●TOBIAS SANDER and GEORG KRESSE — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green’s function formalism from many-body perturbation theory gives access to electronic structure calculation within the quasiparticle picture, as well as provides for calculating optical absorption spectra. Within the traditional ansatz [1], a Bethe-Salpeter like equation for the polarizability is solved. This requires to diagonalize an in general non-hermitian and complex matrix (BSE matrix). Usually, the off-diagonal elements of the BSE matrix are neglected and this is referred to as Tamm-Dancoff approximation. The computational effort can be reduced by using the time-evolution ansatz [2] which avoids the matrix diagonalization. We present a method based on the time-evolution al-

gorithm, that finally avoids storing and diagonalizing the BSE matrix. This leads to a reduction of the scaling w.r.t the system size N from N^5 to N^3 . Finally, we present first results for typical systems.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)

[2] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

MM 52.4 Thu 11:30 TRE Ma

New starting point for the calculation of optical properties — ●IGOR RESHETNYAK^{1,2} and LUCIA REINING^{1,2} — ¹Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — ²European Theoretical Spectroscopy Facility (ETSF)

The Bethe-Salpeter Equation based on Hedin's GW approximation to the self-energy is a powerful approach for describing electron-hole interactions in optical properties and photo-absorption spectra. However, in its current formulation it is both computationally heavy and displays cancellation effects not accounted for analytically. We discuss the sources of these cancellations and the possibility of putting them forward explicitly. We furthermore assess alternative formulations and sets of approximations to the BSE. For each of them we examine its behavior on model systems as well as their computational applicability. Finally we suggest possible directions for further investigations.

MM 52.5 Thu 11:45 TRE Ma

Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles — ●CLAUDIA RÖDL, FRANCESCO SOTTILE, MATTEO GATTI, and LUCIA REINING — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant $O\ 2p$ and localized $Cu\ 3d$ electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

Electron-energy loss and inelastic x-ray scattering experiments yield direct access to the wave-vector- and frequency-dependent loss function $-\text{Im}\ \varepsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q},\omega)$, and, hence, to the screened Coulomb interaction W . We use time-dependent density-functional theory (TDDFT) to calculate the loss spectrum of CuO and discuss the occurring d - d and plasmon excitations. This allows us, by comparing theory and experiment, to assess the quality of the screened Coulomb interaction which is a key quantity for many-body approaches, for instance, *GW* and Bethe-Salpeter calculations.

MM 52.6 Thu 12:00 TRE Ma

Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory — ●CATERINA COCCHI and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

The spurious long-range behavior of time-dependent (TD) density functional theory (DFT) is a well known source of error in describing bound excitons in solids. Remarkably, TD-DFT is often able to capture the optical features of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation. With the example of molecular crystals, we aim at solving the puzzle when and why TD-DFT can be relied on. We answer this question by confronting TD-DFT with many-body perturbation theory (GW and Bethe-Salpeter equation), which is the most accurate methodology to describe optical excitations in solids. Our results are obtained with the all-electron code "exciting" (<http://exciting-code.org>), where all the quantities entering the two formalisms are treated on the same footing [1]. In-depth analysis allows us to identify the shortcomings of TD-DFT in predicting the excitonic spectra of extended systems and to understand when this methodology is capable of providing correct results.

[1] S. Sagmeister and C. Draxl, Phys. Chem. Chem. Phys. 11, 4451 (2009)

MM 52.7 Thu 12:15 TRE Ma

Relativistic Solar Cells — ●PAOLO UMARI¹, EDOARDO MOSCONI²,

and FILIPPO DE ANGELIS² — ¹Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — ²Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy

Hybrid AMX_3 perovskites ($A=Cs, CH_3NH_3$; $M=Sn, Pb$; $X=halide$) have revolutionized the scenario of emerging photovoltaic technologies. Indeed, a rapid evolution led, very recently, up to 15% efficient solar cells. $CH_3NH_3PbI_3$ has so far dominated the field, while the similar $CH_3NH_3SnI_3$ has not been explored for photovoltaic applications, despite the reduced band-gap. Replacement of Pb by the more environment-friendly Sn would facilitate the large uptake of perovskite-based photovoltaics. Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood. Here we develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$, opening the way to new materials design. The different $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$ properties are discussed in light of their exploitation for solar cells, and found to be entirely due to relativistic effects.

MM 52.8 Thu 12:30 TRE Ma

Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS — ●STEFAN WIPPERMANN¹, MARTON VÖRÖS², ADAM GALI³, FRANCOIS GYGI², GERGELY ZIMANYI², and GIULIA GALLI² — ¹Max-Planck-Institute for Iron Research, Düsseldorf — ²University of California, Davis — ³Budapest University of Technology and Economics

We propose that embedding silicon nanoparticles (NP) into amorphous, non-stoichiometric ZnS leads to promising nanocomposites for solar energy conversion. Using *ab initio* molecular dynamics simulations we show that upon high temperature amorphization of the host chalcogenide, sulfur atoms are drawn to the NP surface. We found that the sulfur content may be engineered to form a type II heterojunction, with complementary charge transport channels for electrons and holes, and that sulfur capping is beneficial to lower the nanoparticle gap, with respect to that of NPs embedded in oxide matrices. Our analysis was conducted using density functional theory with local and hybrid functionals and many body perturbation theory at the GW level.

MM 52.9 Thu 12:45 TRE Ma

Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals — ●NGOC LINH NGUYEN¹, GIOVANNI BORCHI¹, ANDREA FERRETTI², ISMAILA DABO³, and NICOLA MARZARI¹ — ¹Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — ²Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — ³Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

We study the photo-electron properties of organic photovoltaic molecules using Koopmans-compliant functionals [1] as well as the Perdew-Zunger self-interaction correction (PZ-SIC) [2] to density-functional theory. A simple method for simulating ultraviolet photo-emission spectra (UPS) of molecules has been implemented. It is based on a plane-wave approximation for the final states to account for the spectra intensities. Our calculations show that Koopmans-compliant functionals provide ionization potentials and electron affinities closely comparable with those obtained by many-body perturbation theory (GW). In addition, we find that UPS spectra computed imposing the Koopmans' condition on the PZ-SIC functional are in remarkable agreement with experimental results.

Refs: [1] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010); [2] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

MM 52.10 Thu 13:00 TRE Ma

Self-consistent dynamical embedding in real space — ●WAEEL CHIBANI¹, XINGUO REN^{1,2}, PATRICK RINKE¹, and MATTHIAS SCHEFFLER¹ — ¹Fritz Haber Institute of the Max Planck Society, Berlin, Germany — ²Key Laboratory of Quantum Information, USTC, Hefei, China

Density-functional theory with its local-density (LDA) and generalized gradient approximations (GGA) is known to fail for localized states. To extend *ab initio* approaches to this domain, we have devised an embedding scheme that facilitates the treatment of the physically im-

portant part of a system with electronic structure methods, that are computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches, i.e. LDA/GGA, in a self-consistent manner. Our scheme is based on the concept of dynamical mean-field theory (DMFT) [1]. However, in contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The

performance of our scheme is demonstrated by treating the embedded region with hybrid functionals for simple bulk systems, e.g. Si or NiO. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. By treating the embedded region with *GW* we were able to improve the band gap using only a small cluster. The effect of self-consistency in *GW* for the embedded region will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**,14 (2006)

MM 53: Topical session: X-ray and neutron scattering in materials science II - Atomic migration studies ranging from neutrons to coherent X-rays

Time: Thursday 11:45–13:15

Location: BAR 205

Topical Talk MM 53.1 Thu 11:45 BAR 205
Atomic migration studies ranging from neutrons to coherent X-rays — ●BOGDAN SEPIOL¹, MARKUS STANA¹, MANUEL ROSS¹, and MICHAEL LEITNER^{1,2} — ¹Universität Wien, Fakultät für Physik, Boltzmannngasse 5, 1090 Wien, Austria — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Numerous properties of materials can be attributed to the movement of single atoms. Understanding the processes involved in atomic transport is therefore of great importance for improving both the fabrication and the stability of materials. Studies of diffusion mechanisms on the atomic scale are, however, particularly challenging. Just a few methods are sensitive to movements on the atomic scale but they are limited to a restricted number of suitable isotopes. Due to these limiting factors it is very difficult or even impossible to apply these methods for studying metastable systems like glasses or nanocrystalline materials on the atomic scale. The advent of modern synchrotron sources opened the way for a new experimental technique which is not subject to these restrictions. I will follow in my talk the development of atomic migration studies ranging from quasielastic neutron scattering, quasielastic Mössbauer spectroscopy, nuclear resonant scattering until the most advanced method for studying dynamics in solid state materials called atomic-scale X-ray photon correlation spectroscopy.

This work was financially supported by the Austrian Science Fund (FWF) P-22402.

MM 53.2 Thu 12:15 BAR 205

Hydrogen motion in LiBH₄ across the structural phase transition — ●LUCA SILVI and WIEBKE LOHSTROH — Forschungsneutronenquelle Heinz Maier-Leibnitz FRM II, Lichtenbergstrasse 1, 85747 Garching, Germany

Lithium Borohydride (LiBH₄) has an intense research activity due to its high hydrogen content (18.4 mass% H₂ and 121.3 kg/m³ of gravimetric and volumetric hydrogen density). The slow sorption kinetics and the high temperatures required for hydrogen exchange are major obstacle for everyday-life applications. In LiBH₄, hydrogen is bonded covalently to a central Boron atom forming a (negatively charged) tetrahedron, and the BH₄ unit bonds ionically to Li ion. By means of Quasielastic Neutron Scattering (QENS), the localized hydrogen motions were investigated as a function of temperature, across the phase structural transition at 380 K. QENS have been performed at the direct time-of-flight neutron spectrometer TOFTOF at FRM-II, and the Elastic Incoherent Structure Factor (EISF) could be determined in a momentum transfer-range up to 4 Å⁻¹. The large dynamical range is essential for the discrimination of different kind of rotational modes. At temperature below the phase transition, 120° rotations occur around the C₃ symmetry axis of the BH₄ unit. As the phase transition is approached, the dynamic of the BH₄ unit changes continuously. At an intermediate state, a tumbling motion of the tetrahedron is observed, while at 413K the hydrogen motion is best described as a diffusion on a surface of a sphere. The results confirm that the structural phase transition is closely linked with the dynamic of the BH₄ units.

MM 53.3 Thu 12:30 BAR 205

Study of Slow Dynamic processes with Depth Resolution — ●OXANA IVANOVA¹, OLAF HOLDERER¹, and MICHAEL MONKENBUSCH² — ¹Jülich Centre for Neutron Science, Forschungszentrum Jülich, Aussenstelle am MLZ, Garching, Germany — ²JCNS-Jülich Centre for Neutron Science, Forschungszentrum Jülich, Jülich, Germany

Neutron spin-echo (NSE) spectroscopy is a scattering technique where

the spin precession of polarized neutrons in magnetic field is used to achieve the highest energy resolution for measuring tiny velocity changes of the neutron during the scattering process. Unlike the other inelastic scattering techniques, such as time-of-flight spectroscopy, NSE measures the intermediate scattering function $S(Q,t)$ in reciprocal space and time directly. Microscopic to macroscopic time range on large and intermediate length scales are covered.

High energy resolution, low background and high stability of the Jülich Neutron Spin-Echo spectrometer (J-NSE) at Heinz Maier-Leibnitz Zentrum (MLZ) makes the instrument suitable for grazing incidence technique. Along with conventional NSE spectroscopy, which enables the measurements in bulk, grazing incidence NSE spectroscopy (GINSES) can be used as dynamic analog to GISANS in order to resolve depth dependent near surface motions. Typical applications of J-NSE include dynamics in soft matter systems (polymers in solution and under confinement, microemulsions, blends, microgels, proteins, membranes, nano-composites) or paramagnetic properties of e.g., spin glasses. Some examples of the recent experiments will be presented.

MM 53.4 Thu 12:45 BAR 205

Microscopic structure of supercooled water studied by x-ray Compton scattering — ●JURI NYROW¹, FELIX LEHMKÜHLER², MIKKO HAKALA³, THOMAS BÜNING¹, INGO STEINKE², AGNIESZKA POULAIN⁴, THOMAS BUSLAPS⁴, METIN TOLAN¹, and CHRISTIAN STERNEMANN¹ — ¹Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — ²Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — ³Department of Physics, University of Helsinki, FI-00014 Helsinki, Finland — ⁴ESRF, 38043 Grenoble Cedex 9, France

The structure of the hydrogen bond network of water at ambient and in supercooled conditions is controversially discussed, e.g. with respect to a mixture of two phases, LDW (low density water) and HDW (high density water). HDW and LDW phases differ fundamentally in respect of the local structure, with the high density phase showing a highly disturbed OH bonding network and the low density phase showing a nearly tetrahedral coordinated water network. Recently inelastic neutron scattering studies reported a disturbance of the water network at slight supercooling. We investigated changes in the local molecular structure in supercooled water for temperatures down to 256 K by x-ray Compton scattering and found evidence for structural changes which will be discussed on the basis of different structure models.

MM 53.5 Thu 13:00 BAR 205

Mechanical properties of mesocomposite silk fibres: viscoelasticity, structural and molecular origin — ●IGOR KRASNOV¹, TYLO SYDLE², MICHAEL M. KOZA², MANFRED BURGHAMMER³, and MARTIN MÜLLER¹ — ¹Helmholtz-Zentrum, Geesthacht, Germany — ²ILL, Grenoble, France — ³ESRF, Grenoble, France

To study the response of silk to a mechanical perturbation we monitor the changes of the microscopic structure of silk as well as the molecular dynamics of the amorphous phase. In order to achieve this goal *in situ* scattering experiments were performed: synchrotron radiation X-rays and cold neutrons were used as probes of the structure and dynamics, respectively. Much attention was devoted to the temporal evolution. Generally, a link between the macroscopic viscoelastic behaviour and the mechanism at the molecular length scales has been established. With our experimental techniques and analyses we could separate the mechanical properties of the crystalline region of silk from those of the amorphous part, as well as show their interplay [1]. Interesting

novel results were also obtained concerning the long-time mechanical relaxation of silk and molecular diffusion processes. Both phenomena exhibit definitive memory effects and can be well described by the models based on fractional calculus. Despite the fact that these

phenomena belong to very different temporal and spatial levels the fractional characteristics of these phenomena are very similar.

[1] Krasnov I., et al. PRL **100**, 048104 (2008)

MM 54: Computational Materials Modelling VIII - Functional materials

Time: Thursday 12:00–13:00

Location: IFW D

MM 54.1 Thu 12:00 IFW D

Modeling lithium-titanium-oxide materials with structural disorder — ●SASKIA STEGMAIER, HENDRIK HEENEN, JÖRG MEYER, CHRISTOPH SCHEURER, and KARSTEN REUTER — Technische Universität München, Germany

Lithium-titanium-oxides are studied intensively owing to their applications as electrode materials in rechargeable lithium-ion batteries.[1] Studies that aim for a better atomic scale understanding of the parameters which influence materials properties and dynamic processes face the challenge that materials like $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO) show structural disorder even in their pure-phase bulk crystal structures. A way to deal with occupational disorder in theoretical studies is the use of supercell structure models. While larger supercells allow for a better representation of the statistical distribution of atom types, they also incur computational costs that quickly become untractable for first principles methods. In consequence, density-functional theory (DFT) calculations on structural features and Li ion diffusion are in practice often carried out for rather small supercell structures. We scrutinize the reliability of such calculations and use force field and DFT methods to evaluate the configuration space for LTO materials with structural disorder.

[1] M. V. Reddy, G. V. Subba Rao, B. V. R. Chowdari, *Chem. Rev.* **2013**, *113*, 5364.

MM 54.2 Thu 12:15 IFW D

Conducting monolayers of Sodium at stacking faults in Silicon — ●BENEDIKT ZIEBARTH^{1,2}, MATOUS MROVEC^{1,2}, CHRISTIAN ELSÄSSER^{1,2}, and PETER GUMBSCH^{1,2} — ¹Fraunhofer IWM, Freiburg, Germany — ²Karlsruhe Institute of Technology, IAM-ZBS, Karlsruhe, Germany

Sodium decorated stacking faults (SFs) in Silicon were identified recently as an origin for potential-induced-degradation failure of solar-cell modules based on crystalline silicon [1]. The SFs were observed to be covered by about one monolayer of Na atoms, and this decoration was interpreted to cause local electrical short-circuits of the p-n-junction in the solar cell. In the present study such a SF in Si decorated with Na was investigated by means of density functional theory in order to elucidate its structural, diffusion and electronic properties. The Na atoms lead to a substantial elongation of Si-Si bonds across the SF. Minimum-energy-path calculations for Na atoms diffusing along the SF yield a strong dependence of the activation barrier on the degree of layer coverage of the SF with Na. In a SF with a half monolayer of Na the barrier is higher than for interstitial Na in bulk Si, whereas in a SF with a full monolayer of Na the barrier is lower by an order of magnitude. Electronic-structure calculations reveal that the Na at the SF cause defect levels in the band gap of Si which are

partially filled and hence lead to electrical conduction along the SF. [1] V. Naumann et al., *phys. stat. sol. (RRL)* **6**, 331-333 (2012).

MM 54.3 Thu 12:30 IFW D

An ab-initio study of muscovite mica — ●ANOOP KISHORE VATTI, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Muscovite mica is the most significant phyllosilicate mineral in the mica series. It is widely used as a substrate in various experiments investigating the structure of water, because it is easily cleaved yielding an atomically smooth surface structure. We perform density-functional theory calculations to study the bulk and surface properties of muscovite mica using both the Local Density Approximation (LDA) and the Generalized Gradient Approximation (PBE-GGA). Inclusion of the semi-empirical dispersion correction of Grimme (vdW-D2) turns out to be essential in order to achieve an accurate description of the system. The structural parameters, elastic constants and electronic structure of muscovite mica will be discussed, as well as the thermodynamic stability of different surface terminations.

MM 54.4 Thu 12:45 IFW D

Modeling the screening in atomically thin layers — ●RALF HAMBACH¹, PHILIPP WACHSMUTH¹, GERD BENNER², and UTE KAISER¹ — ¹Electron Microscopy Group of Materials Science, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — ²Carl Zeiss Microscopy GmbH, Carl-Zeiss-Str. 22, 74447 Oberkochen, Germany

In this joint experimental and theoretical work, we investigate the electronic screening in free-standing, tilted graphene as prototype 2D material. To this end, the momentum-dependent electron energy-loss function has been measured by angular-resolved electron energy-loss spectroscopy up to 40eV using a transmission electron microscope (SALVE-I [1]). Corresponding ab-initio calculations in the framework of time-dependent density-functional theory have been performed using a plane-wave pseudopotential code [2,3]. We find very good agreement between experimental and theoretical results both for in-plane and for out-of-plane momentum transfers.

Starting from our ab-initio calculations, we assess the importance of out-of-plane excitations in the electronic screening and discuss the validity of a two-dimensional description of graphene which is often applied in model calculations by neglecting the extension in perpendicular direction. Finally, we discuss simple dielectric models to describe the anisotropy of graphene and the observed plasmon dispersion.

[1] Kaiser et al, *Ultramicroscopy* **111** 1246 (2011)

[2] AbInit: Gonze et al, *Comp. Mat. Sci.* **25** (2002)

[3] Olevano, Reining, Sottile, <http://www.dp-code.org> (1998)

MM 55: Nanomaterials III - Electronic, magnetic and optical properties

Time: Thursday 12:00–13:15

Location: IFW B

MM 55.1 Thu 12:00 IFW B

Dimension and angle dependence of coercivities and magnetization reversal mechanisms in fourfold ferromagnetic systems — ●TOMASZ BLACHOWICZ¹ and ANDREA EHRMANN² — ¹Silesian University of Technology, Institute of Physics, Gliwice, Poland — ²Niederrhein University of Applied Sciences, Mönchengladbach, Germany

Stability of magnetic states during evolution from saturation to anti-saturation and vice-versa, especially at remanence, belongs to the important issues in examination of magnetic nanosamples. Our presentation gives an overview of different fourfold magnetic wire systems, simulated by Magpar. Wire lengths have been chosen from 30 nm to 70 nm, while single wires have length-to-diameter ratios between 3 and 11. All simulations have been carried out for several angular in-plane directions of the externally applied field, ranging from 0° (parallel to a pair of wires) to 45°. Depending on system dimensions and field orientation, different magnetization reversal mechanisms could be observed as well as changes between stable and instable magnetic states [1].

Intermediate states at vanishing external field, reached by minor loops starting at steps in the hysteresis loop, are of special interest for application in novel data storage media systems. The presentation shows different possibilities to create such states and examines their stability by comparing hysteresis loops, special distribution of magnetization, and exchange energy as function of the externally applied field for a number of sample dimensions and external field angles.

[1] T. Blachowicz, A. Ehrmann, J. Appl. Phys. 113, 013901 (2013)

MM 55.2 Thu 12:15 IFW B

Macro-spin modeling of magnetization reversal processes in systems with different anisotropies — ●ANDREA EHRMANN¹ and TOMASZ BLACHOWICZ² — ¹Niederrhein University of Applied Sciences, Mönchengladbach, Germany — ²Silesian University of Technology, Institute of Physics, Gliwice, Poland

Examinations of magnetic systems by use of a single macro-spin can support understanding magnetization reversal processes in principal. Such a macro-spin model, considering perfectly coherent rotation, can reproduce qualitatively all outstanding features of systems in which magnetization reversal is not based on domain wall processes [1].

A calculation based on constant energy minimization during the reversal process from positive to negative saturation and vice versa has been implemented in PTC(R) Mathcad. In this calculation, a simple macro-spin model describes the coherent rotation of a single magnetic moment (macro-spin) using the total energy density, consisting of different magnetic anisotropies as well as the external magnetic field. Thus, hysteresis loops of the longitudinal and the transverse magnetization component can be calculated. Besides coercive fields and shapes of the longitudinal magnetization loop, the calculation can also be used to detect angular orientations of the sample relative to the external magnetic field for which the transverse signals vanish.

[1] A. Tillmanns, S. Oertker, B. Beschoten, G. Güntherodt, J. Eisenmenger, Ivan K. Schuller: Angular dependence and origin of asymmetric magnetization reversal in exchange-biased Fe/FeF₂(110), Phys. Rev. B 78, 012401 (2008)

MM 55.3 Thu 12:30 IFW B

Plasma assisted gas phase synthesis and high resolution characterization of bimetallic magnetic core-shell nanoparticles —

●MARCEL HENNES¹, ANDRIY LOTNYK¹, and STEFAN G. MAYR^{1,2,3} — ¹Leibniz-Institut für Oberflächenmodifizierung, Leipzig, Germany — ²Translationszentrum für Regenerative Medizin, Leipzig, Germany — ³Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Magnetic nanoparticles (MNPs) can be employed as powerful nanotools in many areas of biology, biophysics and medicine. Therefore, fine tuning of their physical properties is highly desired and can be achieved by controlling their size or shape or by using combinations of materials at the nanoscale. With this background, a setup for synthesis of heterostructured magnetic core-shell nanoparticles (CS-MNPs) relying on optionally pulsed DC plasma assisted inert gas condensation (PA-IGC) has been developed. We demonstrate synthesis of elemental nickel nanoparticles with highly tunable sizes and shapes as well as Ni@Cu CS-MNPs. The particles are characterized with respect to their structural and magnetic properties using AFM, MFM, SEM, HRTEM and EDX measurements. An analytical model is used to describe Cu shell atom deposition on top of Ni-particles in the gas phase. Its predictive power and possible implications for heterostructured NP growth are discussed.

MM 55.4 Thu 12:45 IFW B

Electrical characterization of single FePt nanoparticles — ●ULRICH WIESENHÜTTER¹, DARIUS POHL², BERND RELLINGHAUS², JÜRGEN FASSBENDER¹, and ARTUR ERBE¹ — ¹Helmholtz-Zentrum Dresden Rossendorf, D-01328 — ²Leibniz-Institut für Festkörper- und Werkstofforschung, D-01069

In order to correlate the size and crystallinity of FePt nanoparticles to their electrical properties, single nanoparticles are contacted to electric leads using electron beam lithography. The particles are prepared from gas phase on electron transparent SiN membranes which allow for imaging the electrically investigated particle by means of transmission electron microscopy. The electrical characterization is carried out by recording current-voltage characteristics. As a result, Coulomb-blockade effects were observed at low temperatures which is in agreement with the dimensions obtained from the TEM studies. Individual properties of the particle - electrode junctions, i.e., capacitances and coupling parameters were derived from reconstructed Coulomb-blockade diamonds.

MM 55.5 Thu 13:00 IFW B

Electroluminescent silver surfaces — ●INES CASPERS, JOHANNA KIRSCHNER, TOBIAS HAUG, SEBASTIAN BANGE, and JOHN M. LUPTON — Universität Regensburg, Deutschland

Electrically contacted silver island metal films exhibit electroluminescence after deliberate introduction of a tunneling barrier into the film. The nanoscale barrier is formed by application of a direct current, while the subsequent stable light emission is excited by an alternating current. Most of the observed photons are emitted in the near-infrared region and are detected from small emissive centers located within the tunneling junction. We attribute the phenomenon to an inelastic tunneling process of electrons through the barrier formed between adjacent silver nanoparticles. The tunneling electrons are understood to couple to and excite localized surface plasmons that eventually decay radiatively. The emission polarization is correlated with the dipole formed by two nanoparticles and thus partially polarized with a reduced preference for orientation perpendicular to the tunneling current.

MM 56: Liquid and Amorphous Metals IV

Time: Thursday 11:30–13:00

Location: IFW A

MM 56.1 Thu 11:30 IFW A

Scenarios of structure stabilization in amorphous AlMnCu — ●SYED SAJID ALI GILLANI and PETER HÄUSSLER — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Structural studies of binary amorphous AlMn and AlCu and two different cuts through the ternary AlMnCu show purely amorphous regions, those with additional quasi-crystalline features, as well as those with nano-crystalline inclusions. Our analysis focuses on global resonance effects between two global subsystems, the Fermi gas as one and the static structure as the other one. The global resonances in this case are self-organizing via the exchange of a characteristic momentum, supported by density anomalies, hybridization effects and phase separations. For both, the binary *a*-AlMn as well as the binary *a*-AlCu systems, the corresponding structure factors $S(K)$ show the resonance peaks at $K_{pe} = 2k_F$. They correspond in *r*-space to a spherical-periodic atomic order. The self-organizing processes are limited since e.g. hybridization needs minimal as well as maximal contents of transition metals (here Mn) and changes if we replace the Mn. To go more into details, we go along two cuts through the ternary AlMnCu and so are able to cross the several limits at different compositions. Amorphous AlMnCu seems to be a model system for a deeper understanding of those effects. For one cut we start at *a*-Al₅₀Mn₅₀ and add Cu. A second cut starts from *a*-Al₆₀Cu₄₀, keeps the Cu-content constant and varies both, the Al- as well as the Mn-content. We report on the results.

MM 56.2 Thu 11:45 IFW A

Investigations of temperature-time-transformation behavior of bulk glass forming alloys — ●STEFANIE KOCH^{1,2}, DIETER M. HERLACH^{1,2}, and MARKUS RETTENMAYR³ — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — ²Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum, Germany — ³Otto-Schott-Institut für Materialforschung, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

Isothermal crystallization studies were performed on Zr-based bulk glass forming alloys in the undercooled liquid region between the glass transition and liquidus temperature. The resulting temperature-time-transformation (TTT) diagram for crystallization is used to identify the primary factors influencing their glass-forming ability.

To prevent heterogeneous nucleation on container walls, levitation techniques are used. In this work electrostatic levitation (ESL) is used to melt and undercool samples. Containerless processing is an effective tool for undercooling melts far below their equilibrium melting temperatures. In case of ESL samples in a diameter of 3mm are processed in ultra-high vacuum.

At first an effect of the temperature from which the melt is cooled is observed on the crystallization behavior for Zr-based bulk metallic glasses. A critical temperature is found above which there is an increase in the undercooling and the crystallization time. To determine the TTT diagram, isothermal experiments were performed.

This work is supported by DLR Space Management.

MM 56.3 Thu 12:00 IFW A

Indication for a liquid-liquid phase transition during ultrafast heating of metallic glasses — ●STEFAN KÜCHEMANN¹, NORBERT MATTERN², and KONRAD SAMWER¹ — ¹Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — ²Leibniz Institut für Festkörper- und Werkstoffprüfung Dresden, 01171 Dresden, Germany

Although the origin of the dramatic change of the dynamics in the supercooled liquid region of metallic glasses has been studied since many years, there is still no conclusive explanation for this behavior. The incipient crystallization process limits the number of possible techniques which can be used to study the supercooled liquid region of metallic glasses. In this contribution, we used an ultrafast capacitor discharge in order to heat up metallic glasses homogeneously above the glass transition temperature with typical heating rates of the order of 106 K/s [1]. For our measurements, we used melt-spun ribbons of nominal composition of Zr₆₅Cu_{27.5}Al_{7.5}. At high temperatures, we studied the specific heat as well as structural changes during the crystallization at different temperatures. Therefore, X-ray measurements have been per-

formed at P07 beamline of PETRA III at DESY. A newly developed chopper system has been used in order to enhance the temporal resolution of the 2D detector from 15 Hz up to 195 Hz. The observations will be discussed in the framework of a liquid-liquid phase transition. Financial support by DFG within SFB 602 is gratefully acknowledged.

[1] William L. Johnson et al., Science 332, 828 (2011)

MM 56.4 Thu 12:15 IFW A

Thermal Conductivity of Superconducting Bulk Metallic Glasses in the Temperature Range between 6 mK and 300 K — ●DANIEL ROTHFUSS¹, ANDREAS REISER¹, ANDREAS FLEISCHMANN¹, UTA KÜHN², and CHRISTIAN ENSS¹ — ¹Kirchhoff-Institute for Physics, Heidelberg University, INF 227, 69120 Heidelberg — ²IFW Dresden, Institute for Complex Materials, P.O. Box 270116, 01171 Dresden

Bulk metallic glasses (BMG) are a new and very interesting kind of amorphous materials. Measuring the thermal conductivity provides the possibility to probe the fundamental interactions governing the heat flow in solids. We present the first measurements of the thermal conductivity of two superconducting BMGs in the temperature range from 6 mK to 300 K. Our results show that the thermal conductivity of BMGs can be described by two independent contributions based on conduction electrons and phonons. Above the critical temperature T_c the part based on conduction electrons is determined by defect scattering and reduces rapidly below T_c . Sufficiently far below T_c the thermal conductivity is based on the part of the phonons and can be described by their resonant scattering with tunneling systems. Above T_c the contribution of the phonons can be described successfully within a novel model considering not only electrons and phonons but also localized modes as scattering centres. At ultralow temperatures a new contactless measuring technique was used, which is based on optical heating and paramagnetic temperature sensors that are read out by a SQUID magnetometer.

MM 56.5 Thu 12:30 IFW A

Heat flow analysis of amorphous solids using dynamic differential scanning calorimetry (DDSC) — ●BIRTE RIECHERS¹, RANKO RICHERT², CARSTEN MAHN¹, and KONRAD SAMWER¹ — ¹Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland — ²Department of Chemistry and Biochemistry, Arizona State University, USA

Relaxation modes, especially their detailed description and understanding, play a captivating role for physicists working with glassy matter. One of many interesting aspects is the temperature dependence of the relaxation mode distribution, and of their relaxation times, which can be explored by DDSC. Therefore, the heat response of amorphous PdCuSi and PMMA is analyzed by applying a periodic triangular excitation of temperature below the glass transition temperature. Though only odd harmonics contribute to the excitation function, i.e. temperature, also even harmonics are seen in the response function, i.e. heat flow. This non-linear behavior gives information about the energy transfer to excited relaxation modes due to temperature variation. Moreover, the change in specific heat of even harmonics offers insight into temperature dependent relaxation times of excited modes.

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

MM 56.6 Thu 12:45 IFW A

High-resolution laser dilatometry applied to volume equilibration phenomena in bulk metallic glasses — ●MARTIN LUCKABAUER¹, UTA KÜHN², JÜRGEN ECKERT², and WOLFGANG SPRENGEL¹ — ¹Institut für Materialphysik, Technische Universität Graz, Austria — ²Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Germany

The slowing down of molecular or atomic motion occurring at the calorimetrically determined glass transition temperature T_g upon cooling complicates the access of kinetic processes at lower temperatures. However, possible changes around or below T_g regarding the structural dynamics are believed to yield key parameters in understanding the glass transition. In this talk some insight on how to examine the equilibration processes in the far sub- T_g regime will be given applying the method of high-resolution laser dilatometry. This technique involves contactless measurements with a 2-beam Michelson laser-

interferometer capable of accessing volume equilibration time constants of up to $1 \cdot 10^6$ s with a length change resolution of up to 10 nm. In addition the dynamical change of the instantaneous thermal expansion coefficient during volume equilibration can be studied simultaneously. Experimental results regarding changes in the volume equilibration

processes upon approaching the glass transition from lower temperatures are presented. Moreover, the possibility of using the thermal expansion coefficient as an indication of the equilibration state of the material is discussed. Financial support by the Austrian Science Fund (FWF) is appreciated (project P22645-N20).

MM 57: Invited Talk (Hauptvortrag) Hono

Time: Thursday 15:00–15:30

Location: BAR 205

Invited Talk MM 57.1 Thu 15:00 BAR 205
Toward the development of Dy-free high coercivity Nd-Fe-B permanent magnets — ●KAZUHIRO HONO, HOSSEIN SEPEHRI-AMIN, and TADAKATSU OHKUBO — National Institute for Materials Science

Due to the recently-emerged concern about the scarce resource of heavy rare earth (HRE) elements, finding a way to increase the coercivity of Nd-Fe-B magnets without using Dy has become the center of permanent magnet research in Japan. In this talk, we will

give an overview on our recent progresses toward the development of high coercivity Dy-free Nd-Fe-B permanent magnets. Based on the microstructure-coercivity relationships investigated by multi-scale characterization with SEM, TEM and atom probe tomography (APT), we have studied the microstructure-coercivity relationships of Nd-Fe-B based magnets systematically. Comparing the results with micromagnetic simulations, we discuss the way to achieve a coercivity higher than 2.5 T in Nd-Fe-B based permanent magnets without HRE.

MM 58: Topical session: X-ray and neutron scattering in materials science III - Real-time insights into fast heat treatment processes using diffraction methods

Time: Thursday 15:45–17:15

Location: BAR 205

Topical Talk MM 58.1 Thu 15:45 BAR 205
Real-time insights into fast heat treatment processes using diffraction methods — ●JENS GIBMEIER¹, VLADIMIR KOSTOV¹, FABIAN WILDE², PETER STARON², ARNE KROMM³, THOMAS KANNENGIESSER³, and ALEXANDER WANNER¹ — ¹KIT, Inst. of Applied Materials, Karlsruhe, Germany — ²Helmholtz-Center Geesthacht, Inst. of Mat. Res., c/o DESY, Hamburg, Germany — ³BAM Federal Inst. for Mat. Res. and Testing, Berlin, Germany

Laser surface hardening and related processes are viable techniques for surface integrity optimization of technical components. Although, the techniques are standard processes in industrial applications, process optimization is essentially based on simulation and on characterization after material processing. Moreover, the simulations often lack in an adequate accuracy, since the models are still deficient. Knowledge about the phase transformation kinetics and about the evolution of local (residual) stress distributions is of essential importance for the optimization of the surface hardening process and hence, for the tailoring of the treated surface layers. A considerable progress can be achieved when a real-time insight into these local short-time heat treatment processes can be gained. By this means process comprehension can be achieved as well as a proper validation of the simulation models can be offered. Here, different set-ups for real-time monitoring of phase transformation as well as stress evolution during fast heat treatment processes by means of synchrotron X-ray diffraction will be presented. Successful application for laser surface hardening and arc welding will be shown.

MM 58.2 Thu 16:15 BAR 205
Texture evolution of YCu deformed by high pressure torsion — ●AURIMAS PUKENAS¹, ANDY ESCHKE¹, WERNER SKROTZKI¹, CHRISTINE TRÄNKNER¹, JELENA HORKY², and MICHAEL ZEHETBAUER² — ¹Institut für Strukturphysik, TU Dresden, Dresden, Germany — ²Fakultät für Physik, Universität Wien, Wien, Austria

YCu is an intermetallic compound with B2 type crystal structure which is ductile at ambient temperature and pressure. Polycrystalline YCu discs were subjected to high pressure torsion (HPT) at a confining pressure of 8 GPa from room temperature up to 300°C. In HPT the deformation of the sample is inhomogeneous along the radial direction. Due to this shear strain gradient, a texture gradient is observed. The texture was measured locally as a function of shear strain by X-ray microdiffraction. The intensity and deviation from the ideal positions of the typical bcc texture components will be discussed and compared to NiAl, another B2 intermetallic compound which is brittle at ambient temperature and pressure conditions.

MM 58.3 Thu 16:30 BAR 205
Application of in-situ high-energy X-ray diffraction and small-angle scattering for the understanding and develop-

ment of advanced intermetallic multi-phase γ -TiAl based alloys — ●EMANUEL SCHWAIGHOFER¹, ANDREAS STARK², PETER STARON², BORIANA RASHKOVA¹, THOMAS LIPPMANN², NORBERT SCHELL², HELMUT CLEMENS¹, and SVEA MAYER¹ — ¹Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Austria — ²Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany

Advanced intermetallic γ -TiAl based alloys, e.g. TNM alloys with a nominal composition of Ti-43.5Al-4Nb-1Mo-0.1B-(0-1)C,Si (in at.%), are predestined for high-temperature (HT) application as turbine blades and turbocharger wheels in modern combustion engines. To improve their HT-potential, state-of-the-art methods based on high-energy monochromatic synchrotron radiation were applied combined with an adapted quenching and deformation dilatometer in order to study equilibrium and non-equilibrium phase transformations, hot-deformation behavior, texture evolution as well as carbide precipitation kinetics. Complementary real-space imaging by means of scanning and transmission electron microscopy as well as lab-scale XRD and hardness testing were performed for verification. In this talk, selected topics of the use of in-situ synchrotron scattering techniques, i.e. diffraction and small-angle scattering, conducted at HZG-operated beamlines HARWI II and HEMS at the synchrotron facility DESY, Germany, are discussed for a deeper understanding of this class of alloys.

MM 58.4 Thu 16:45 BAR 205
In situ high energy X-ray diffraction for analyzing the local stress distribution and microstructure in the chip formation zone during orthogonal cutting of steel C45E — ●KATRIN BRÖMMELHOFF¹, STEFFEN HENZE², ROBERT GERSTENBERGER², TORBEN FISCHER³, NORBERT SCHELL³, ECKART UHLMANN², and WALTER REIMERS¹ — ¹TU Berlin, Materials Science and Technology-Metallic Materials, Ernst-Reuter-Platz 1, 10587 Berlin, Germany — ²TU Berlin, IWF, Pascalstr. 8-9, 10587 Berlin, Germany — ³Helmholtz-Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht, Germany

The stress distribution in the chip formation zone during cutting is an asked question in the field of manufacturing technology and is required for a fundamental understanding of the chip formation process. New synchrotron facilities with high photon flux provide the opportunity to measure the local strains with a high spatial resolution. Therefore, the steep stress gradients in the chip formation zone can be analyzed. Performing in situ high energy synchrotron X-ray diffraction during orthogonal cutting at the HEMS beamline (PETRA III/Hamburg), the beam size and therefore the measuring positions could be reduced to 0.02 mm x 0.02 mm. The stress distribution exhibits steep stress gradients and shows significant dependencies on the cutting parameters and a strong change of the microstructure was observed, namely a reduction of domain sizes and the development of a shear texture. The results of these in situ experiments serve to evaluate and extend

existing chip formation models and will be used for the optimization of FEM (Finite Element Method) cutting simulations.

MM 58.5 Thu 17:00 BAR 205

Synchrotron radiation based non-destructive investigation of Neolithic and Early Bronze Age axe — •LEIF GLASER¹, MECHTILD FREUDENBERG², KAREN APPEL¹, MANUELA BORCHERT¹, JOERN DONGES¹, ANDREW KING³, THOMAS LIPPMANN⁴, ANDRE ROTHKIRCH¹, and NORBERT SCHELL⁴ — ¹DESY, Hamburg, Germany — ²Stiftung Schleswig-Holsteinische Landesmuseen, Schloß Gottorf, Schleswig, Germany — ³ESRF, Grenoble, France — ⁴HZG, Geesthacht, Germany

To understand the historic production methods bronze axe replicas were cast and treated using replicated stone tools for metalworking.

To understand techniques for smoothing the surfaces, hardening the cutting edge, and cutting or embossing the elaborate ornaments of the surface, repeated investigations, using non-destructive SR-based techniques, as XRF and XRD in transmission and reflectance geometry were performed on the replicas and original ancient axes.

Based on our experiments the reproduction techniques for making replicas could be improved, while on the other hand some historic references could be identified as historic forgeries, but forgeries nonetheless. Further experiments concerning the actual casting process are ongoing, with emphasis on most likely casting inflicted variable stoichiometric bronze distribution within the individual object. Some replica were cast at the Howadtsche Metallgiesserei Kiel using modern casting techniques, others at the Archaeological Landesmuseum Schloß Gottorf using historic methods and tools only, while the experiments were performed in Hamburg at DESY.

MM 59: Computational Materials Modelling IX - Ferroelectrics

Time: Thursday 15:45–17:45

Location: IFW D

MM 59.1 Thu 15:45 IFW D

Ferroelastic Switching of Doped Zirconia – First-Principles Insights — •CHRISTIAN CARBOGNO^{1,2}, CARLOS G. LEVI¹, CHRIS G. VAN DE WALLE¹, and MATTHIAS SCHEFFLER^{1,2} — ¹Materials Department, University of California, Santa Barbara, USA — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

ZrO₂ based ceramics play a pivotal role for thermal barrier coatings in gas and propulsion turbines. The phase stability required for these applications is typically achieved by Y-doping, which however also results in an undesirable degradation of toughness. Recently, high phase stability and toughness has been achieved by co-doping such Y-stabilized ZrO₂ (YSZ) with Ti (TiYSZ) [1]. We use density-functional theory to investigate these effects by inspecting the underlying structural dynamics. Our calculations reveal that the minimum-energy path (MEP) for the tetragonal-to-cubic phase transformation differs significantly from the path discussed in literature [2]. We show that the correct MEP involves *ferroelastic switches*, i.e., the realignment of the tetragonality along a different cartesian direction. We inspect how (co-)dopants affect these *ferroelastic switches*, which are typically considered to be the primary toughening mechanism in these compounds [1]. Hence, our calculations shed light on the atomistic mechanisms that determine the dynamics and the high-temperature properties of YSZ and TiYSZ.

[1] T. A. Schaedler, O. Fabrichnaya, and C. G. Levi, *J. Eur. Ceram. Soc.* **28**, 2509 (2008).

[2] S. Fabris, A. T. Paxton, and M. W. Finnis, *Acta Materialia* **50**, 5171 (2002).

MM 59.2 Thu 16:00 IFW D

Microscopic description of BaTiO₃ and related materials near the ferroelectric phase transition — •GIOVANNI PIZZ¹, ANDREA CEPPELLOTTI¹, SAMED HALILOV², BORIS KOZINSKY³, MARCO FORNARI⁴, and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials, EPFL (CH) — ²Department of Materials Science and Engineering, MIT (USA) — ³Robert Bosch LCC Research and Technology Center, Cambridge (USA) — ⁴Dept. of Physics, Central Michigan University (USA)

Ferroelectric materials like BaTiO₃ have been used for decades in a broad range of technological applications (capacitors, gate dielectrics, IR detectors, holographic memories, ...). However, there is still significant debate in the literature concerning the microscopic behavior of these materials, in particular near the paraelectric-ferroelectric phase transition. In BaTiO₃, Ti displacements with respect to the center of the oxygen cage create local dipole moments that are at the origin of the finite polarization in the ferroelectric states. However, these perovskites display a complex energy landscape with multiple local minima. As a result, local finite dipoles exist even in the paraelectric cubic phase, contrary to what is often assumed in simulations. In order to clarify the microscopic behavior of these materials, we perform total-energy calculations to systematically and automatically explore their energy landscape, together with ab-initio molecular dynamics calculations to assess the driving mechanisms for the formation of the different phases and to understand the differences among different structurally similar materials.

MM 59.3 Thu 16:15 IFW D

Polarization rotation at the ferroelectric domain walls of PbTiO₃ and PZT — •ANAND CHANDRASEKARAN^{1,2}, DRAGAN DAMJANOVIC², NAVA SETTER², and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — ²Ceramics Laboratory, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Polarization rotation and domain wall mobility are two key factors driving the development of state-of-the-art piezoelectric and ferroelectric devices. Ferroelectric domain walls in PbTiO₃ (PT) are thought to be predominantly of the 'Ising type', where the polarization does not rotate but diminishes in magnitude close to the domain wall. However, our first-principles calculations show how tensile strains drastically increase polarization rotation in the vicinity of domain walls, that thus acquire both Néel and Bloch character. Large-scale calculations on PT and ordered lead zirconate titanate (PZT) show that the Bloch and Néel components of the polarization are long ranged, while the Ising component is short ranged and decays over 2-3 unit cells. Our analysis points to the possibility of tuning domain wall thickness through strain engineering. Such rotations enhance domain mobility through a reduction in the barrier energy for polarization reversal. Interestingly, the addition of Zr to PT delivers the required tensile strains, thus leading to the enhanced properties observed at the morphotropic phase boundary in PZT.

15 min break

MM 59.4 Thu 16:45 IFW D

Study of nonmagnetic and ferromagnetic fcc cerium with one-electron methods — •FABIEN TRAN, FERENC KARSAI, and PETER BLAHA — Vienna University of Technology, Vienna, Austria

Density functional theory was used to study at low temperature the α and γ phases of cerium which were identified as the nonmagnetic and ferromagnetic solutions, respectively, that we could stabilize in our calculations. Four different levels of approximations for the exchange-correlation energy were used: LDA, PBE, PBE+ U , and YS-PBEh. The latter two contain an adjustable parameter, the onsite Coulomb repulsion parameter U for PBE+ U and the fraction α_x of Hartree-Fock exchange for YS-PBEh, which were varied in order to study their influence on the results. It is concluded that while a small value of U or α_x leads to the correct trend for the stability ordering of the two phases, larger values are necessary for a better (but still not very satisfying) description of the electronic structure.

MM 59.5 Thu 17:00 IFW D

Comparison of transition path sampling and metadynamics for the study of solid-liquid interface properties — •DANIEL SÖPU, XUEYONG PANG, JUTTA ROGAL, REBECCA JANISCH, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, 44801, Bochum

During solid-liquid phase transformation the kinetics of nucleation and growth are determined to a large extent by interfacial properties. Of particular interest are the interface free energy, the interface mobility and the anisotropy of these quantities. To extract interface proper-

ties from experiment is difficult and likewise atomistic modeling of these properties is challenging and requires sophisticated techniques. Here, we present a comparison of two techniques to study solid-liquid interface properties in Al, namely transition path sampling and metadynamics. Transition path sampling explores transition state regions and generates an ensemble of reactive trajectories that contain the full dynamical information of the phase transformation. Metadynamics is a non-equilibrium molecular dynamics simulation method which reconstructs the free energy surface of the phase transition by adding a time dependent bias potential. We compare and contrast the two methods and for which properties of the solid-liquid transformation each of the methods is most applicable.

MM 59.6 Thu 17:15 IFW D

Crystal structure prediction of materials in the BCNOP system at high pressure — ●ZAMAAN RAZA and MARCO SAIITA — Université Pierre et Marie Curie, Paris, France

The structure and properties of crystals containing light elements with no d- and f-electrons is often thought to be well understood, yet they frequently display unexpected characteristics when subjected to high pressures. We study the formation of novel binary and ternary compounds in the BCNOP system, at a wide range of temperatures and pressures. Examples of such systems include the ternary B-N-O, B-C-O and C-N-O systems, which are poorly understood even at ambient conditions.

In this work, we seek a better understanding of the physical and chemical phenomena occurring at high temperatures and pressures in such systems of light elements, and search for novel phases with industrially important properties, such as superhardness, superconductivity and high energy density. This presentation focuses on the theoretical side, and on what is regarded as one of the most difficult problems in the physical sciences, crystal structure prediction. The problem arises from the fact that the configurational space increases exponentially in size with the number of atoms in the system, making searches for

the ground state on most potential energy surfaces intractable. To this end, we use two different approaches towards structure prediction, namely random structure searching using the AIRSS method (*J. Phys. Condens. Mat.* **23**:53201, 2011) and evolutionary algorithms as implemented in the USPEX suite (*Comp. Phys. Comm.* **175**:713, 2006).

MM 59.7 Thu 17:30 IFW D

Localized Resolution of Identity: Accurate and efficient evaluation of the coulomb operator for advanced functionals — ●ARVID CONRAD IHRIG, JÜRGEN WIEFERINK, IGOR YING ZHANG, SERGEY LEVCHENKO, MATTI ROPO, PATRICK RINKE, VOLKER BLUM, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

A key component for high-level correlation methods is the Coulomb operator, which requires the evaluation of four-center Coulomb integrals. For numeric atom-centered orbitals, as used in the all-electron code FHI-aims [1], the four-center integrals are most efficiently evaluated with the “Resolution of Identity” (RI), which expands basis-function products in an auxiliary basis. In this contribution we show the practical applicability of a localized RI-variant (“RI-LVL”), which expands products of basis functions only in the subset of those auxiliary basis functions which are located at the same atoms as the basis functions. We demonstrate the accuracy of RI-LVL for exact exchange in HF and PBE0, and also for correlation methods like MP2 and RPA for the S22 test set[2] of weakly interacting dimers. The error relative to the established RI can be converged in a systematic way by augmenting the auxiliary basis set with additional basis functions of increasing angular momentum. We also show that RI-LVL exhibits a superior scaling with system size, both in terms of computational time and memory requirements.

- [1] V. Blum *et al.*, *Comput. Phys. Commun.* **180**, 2175 (2009)
 [2] P. Jurečka *et al.*, *Phys. Chem. Chem. Phys.* **8**, 1985 (2006)

MM 60: Nanomaterials IV - Deformation and mechanical properties

Time: Thursday 15:45–17:00

Location: IFW B

MM 60.1 Thu 15:45 IFW B

Deformation of nanoporous gold: the importance of topology — ●BAO-NAM D. NGO^{1,3}, KARSTEN ALBE², and JÖRG WEISSMÜLLER^{1,3} — ¹Institut für Werkstofforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Darmstadt, Germany — ³Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

We present a molecular dynamics study on the influence of the topology on the mechanical properties of nanoporous gold. Following a suggestion by N. Huber *et al.* [1], we study a highly symmetric diamond-like structure and compare it to a disordered structure, both having comparable relative density, feature size, and surface area. The random sample shows zero lateral expansion to a certain point under compression and noticeable lateral contraction in tension. Plasticity happens immediately upon compression, followed by strain hardening of material due to dislocation activity. In line with continuum modeling, the symmetric structure shows appreciable lateral strain in both compression and tension. It also shows clear elasticity before yielding, with similar elastic modulus in both test modes. Appreciable dislocation activity in compression is observed only at very large strain. Other relevant mechanical properties are also investigated, suggesting that topology can strongly affect nanoporous mechanical behavior.

[1] N. Huber *et al.*, *Scaling Laws of Nanoporous Metals under Uniaxial Compression*; in preparation (2013).

MM 60.2 Thu 16:00 IFW B

Glass-like characteristics of grain-boundary (GB) mediated plasticity in nanocrystalline (NC) PdAu alloys — ●ANDREAS LEIBNER, MANUEL GREWER, CHRISTIAN BRAUN, JONAS HEPPE, and RAINER BIRINGER — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2 2, 66123 Saarbrücken

There is ample evidence that at the low end of the nanoscale (<10nm), plastic deformation of NC metals manifests among other mechanisms

in shear transformations (ST) that are confined to the core regions of GBs. On the other hand ST are the generic flow defect of metallic glasses. Therefore, it is in order to compare the deformation parameters of NC metals with appropriate counterparts in bulk metallic glasses (BMG).

Here we present a systematic investigation on the elastic properties and plastic behavior of NC PdAu with varying Au concentration and compare our results with solid solution strengthening / softening effects so far observed in nanoscale materials. However, drawing a conclusion, we emphasize an analogy to the deformation behavior in BMG.

MM 60.3 Thu 16:15 IFW B

A comparative study of the mechanical behavior of nanocrystalline metals and bulk metallic glasses using shear compression specimen — ●CHRISTIAN BRAUN, MANUEL GREWER, and RAINER BIRINGER — 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 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. In BMGs, increasing load causes percolation of shear transformations that leads to shear band formation and concomitant strain localization followed by catastrophic failure. On the other hand, in nc metals the deformation seems to be carried by shear transformations distributed across the network of grain boundaries. Instead of catastrophic failure through shear banding, nc metals at the low end of the nanoscale even exhibit strain hardening. We will discuss in detail the similarities and dissimilarities of the deformation behavior of nc Pd90Au10 and the BMG Pd40Ni40P20 under the same loading conditions.

MM 60.4 Thu 16:30 IFW B

Ultra high stresses in thin Nb-H films — ●MAGNUS HAMM, VLADIMIR BURLAKA, STEFAN WAGNER, and ASTRID PUNDT — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Mechanical stress influences different material properties. Some examples are the change of the critical temperature [1], the change of the electromotoric force [2] or changes in the energy-band structure [3]. For thin metal films clamped to a rigid substrate, hydrogen absorption on interstitial lattice sites results in compressive mechanical stress. Up to -3.4 GPa have been measured by Laudahn et al. for Nb-films.[4] While for low concentrations the stress increases linearly with the hydrogen content, the stress increase is reduced by the creation of dislocations, for higher concentrations. As suggested by Nörthemann et al.[5] the mechanical stress evolution depends on the film thickness: Below a critical thickness of the film the formation of dislocations even becomes energetically unfavorable. It is shown that below this critical thickness the stress increases to very high values. This observed stress change is reversible.

Financial support by the DFG via project PU131/12-1 is gratefully acknowledged.

- [1] J. Weissmüller and C. Lemier, *Philos. Mag. Lett.* 80:6 (2000)
- [2] R. Kirchheim, *Acta metall.* 1:34 (1986)
- [3] R. People, *IEEE J. Quantum Electron.*, 22:6 (1986)
- [4] U. Laudahn et al., *J. Alloys Compd.* 293-295:20 (1999)
- [5] K. Nörthemann and A. Pundt, *Phys. Rev. B* 78:1 (2008)

MM 60.5 Thu 16:45 IFW B

Processing of Ti/Al light-weight composite sheets via accumulative roll bonding and differential speed rolling — ●JAN ROMBERG^{1,2}, JENS FREUDENBERGER^{1,3}, JULIANE SCHARNWEBER⁴, TOM MARR¹, JÜRGEN ECKERT^{1,2}, WERNER SKROTZKI⁴, and LUDWIG SCHULTZ^{1,2} — ¹IFW Dresden, Dresden, Germany — ²TU-Dresden, Institut für Werkstoffwissenschaft, Dresden, Germany — ³TU-BA Freiberg, Institut für Werkstoffwissenschaft, Freiberg, Germany — ⁴TU-Dresden, Institut für Strukturphysik, Dresden, Germany

Severe plastic deformation (SPD) techniques facilitate the generation of ultra-fine grained metals and, therefore, increase strength and ductility. Among the SPD techniques accumulative roll bonding (ARB) is the only one that facilitates the creation of semi-finished products of reasonable size. In addition, composite materials can be produced by means of ARB. The aim of this study is to create fine laminar Ti/Al composite sheets by means of ARB. Literature discusses the effect of differences in yield stress and presents opportunities of further processing in spite of necked Ti layers. However, previous research have not noticed that the only precondition to avoid necking is sufficient strain hardening. We discuss approaches to increase the strain hardening by means of intermediate heat treatment, the effect of increase of the strain rate and differential speed rolling. The effect of this means on grain size, strength and texture development is shown. It can be expected that further classes of composite materials and non equilibrium solid solutions will be created with the help of the presented results.

MM 61: Liquid and Amorphous Metals V - Structure and structure formation

Time: Thursday 15:45–17:15

Location: IFW A

MM 61.1 Thu 15:45 IFW A

Crystal growth behavior of undercooled silicon melts — ●DANIEL SIMONS¹, PIERRE-YVES PICHON^{1,2}, and DIETER HERLACH¹ — ¹DLR, Institut für Materialphysik im Weltraum, 51170 Köln — ²RGS Development B.V., Bijlvestaal 54 A 1721 PW, Broek op Langedijk, Netherlands

Electromagnetic levitation technique is used to containerless undercool and solidify pure silicon melts. Due to the avoidance of heterogeneous nucleation on container walls large undercoolings up to 320 K below the melting temperature of pure Si, 1685 K, are achieved. The velocity of the crystal growth is measured as a function of undercooling by recording the propagation of the solidification front with a high speed camera. Maximum velocities of 12 m/s are measured at largest undercooling. The high speed video frames give also information of the morphology of the growth front. Plate-like crystals, isolated dendrites, and smaller dendrites at low, moderate and high undercooling temperatures are observed. The plate like crystals morphology is the result of the faceting of the solid-liquid interface at low undercooling. By increasing the undercooling, the solid-liquid interface roughens at the atomic scale, and metallic-like dendrite growth becomes occurs. This effect is identified as kinetic roughening of a smooth solid-liquid interface.

MM 61.2 Thu 16:00 IFW A

Dynamics of wetting and solidification for silicon droplet impacting a cold substrate — ●PIERRE-YVES PICHON^{1,2}, DANIEL SIMONS¹, DIETER HERLACH¹, and AXEL SCHÖNECKER² — ¹DLR, Institut für Materialphysik im Weltraum, Köln, Germany — ²RGS Development B.V., Bijlvestaal 54 A 1721 PW, Broek op Langedijk, The Netherlands

The topic of this work is to examine the wetting dynamics of liquid silicon droplet during the impact on a cold substrate under well controlled conditions. This is motivated by the unusual behavior of the silicon-mold interaction during the crystallization of silicon wafers in the ribbon-growth-on-substrate (RGS) silicon casting process. Silicon droplets were melted in an electromagnetic levitation tool and released so as to impact a cold substrate with a defined amount of kinetic energy. The substrate temperature, wetting properties and roughness were controlled. During the spreading of the droplet on the substrate, the contact line velocity and the dynamic contact angle were recorded with a high speed camera. After the experiment, the interface between the solidified drop and the substrate was analyzed by microscopy. It was found that solidification and wetting strongly interact at the mov-

ing contact line. For example at lower substrate temperature, solidification prevents the system to reach the steady state wetting angle, because attachment kinetics of the atoms to the substrate is diffusion limited: solidification blocks the progression of the contact line. This can explain the behavior of the silicon in the RGS system and gives directions for further improvement of the process.

MM 61.3 Thu 16:15 IFW A

Spatial Distribution of Icosahedra in a Cu-Zr metallic glass — ●JÉRÔME ZEMP¹, MASSIMO CELINO², BERND SCHÖNFELD¹, and JÖRG F. LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — ²ENEA, C. R. Casaccia, Rome, Italy

Topological order in Cu₆₄Zr₃₆ metallic glass was studied by Molecular Dynamics simulations. Structure-specific nearest-neighbor histograms were used to highlight the unique role of Cu-centered icosahedra as compared to other types of Voronoi polyhedra: In both, the glassy and supercooled liquid temperature regime, only icosahedra show a distinct tendency to form superclusters, which is expressed by the strength of the first peak in the Cu-Cu nearest-neighbor histogram. The spatial distribution and interconnectivity of icosahedra were studied as a function of cooling rate and compared to a homogeneous icosahedra distribution. Thermal vibrations were avoided by considering the corresponding inherent structures. Chemical short-range order and potential energy will be discussed as possible reasons for clustering.

MM 61.4 Thu 16:30 IFW A

ASAXS on NiPB amorphous nanograin material — ●SÖREN GAYER¹, ULLA VAINIO¹, VIKRAM RAGHUWANSHI², ARMIN HOELL², ANDREAS SCHREYER¹, and JIXIANG FANG³ — ¹Helmholtz-Zentrum Geestacht, Geesthacht, Germany — ²Helmholtz-Zentrum Berlin, Berlin, Germany — ³Xi'an Jiaotong University, Xi'an, China

An exhaustive understanding of new materials includes a description of the internal structure. As for the class of amorphous nanograin materials, this structure includes inhomogeneities both in density and chemistry. They are produced by compressing nanometer-sized amorphous particles with high pressures. To investigate their structure (anomalous) small-angle X-ray scattering, (A)SAXS, is a good method, sensitive to density and, in the case of ASAXS, chemistry differences.

The nanoparticles for the investigated samples were created by chemical reduction of compounds containing Ni, P and B in solution. The then dried precipitates were compressed with pressures ranging from 0.5 to 4.0 GPa to form thin disks. Due to the chemical reduc-

tion, interfaces were already formed within the relatively large particles during their synthesis.

Measurements were performed at the ASAXS station (7T-MPW-SAXS) at the synchrotron source BESSY II. The measured SAXS curves were fitted with different models to determine sizes and density differences of the substructures. The structural models were then tested with the Akaike information criterion to select the best of them.

MM 61.5 Thu 16:45 IFW A

In-situ XRD studies of Cu-Zr alloys in amorphous, liquid and crystalline state — ●OLGA SHULESHOVA¹, IVAN KABAN^{1,2}, JOZEF BEDNARCIK³, DIRK HOLLAND-MORITZ⁴, JAN GEGNER⁴, FAN YANG⁴, JUNHEE HAN¹, NORBERT MATTERN¹, and JÜRGEN ECKERT^{1,2} — ¹IFW Dresden, Institute for Complex Materials, 01171 Dresden, Germany — ²TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — ³DESY Photon Science, 22607 Hamburg, Germany — ⁴DLR, Institut für Materialphysik im Weltraum, 51170 Köln, Germany

Structure and phase formation in the glass-forming Cu-Zr alloys have been studied *in situ* by high energy synchrotron X-ray diffraction. Heating of the glassy ribbons was carried out with a Linkam hot-stage, while the equilibrium and undercooled liquid alloys were studied with electrostatic levitation technique. Depending on the initial state (either amorphous or liquid), different sequences of crystalline phase

formation have been observed. Analysis of the total pair distribution functions revealed larger differences between the crystalline and parent liquid phase for the alloys with relatively simple (cubic) phase nucleating from the melt, comparing to those where complex crystalline structures are formed. This is thought to indicate distinctions in crystal nucleation and/or growth rates depending on alloy composition, implying different mechanisms that govern glass formation in Cu-Zr system.

MM 61.6 Thu 17:00 IFW A

Surface tension of liquid Al-Au alloys — ●GERHARD KOLLAND and JÜRGEN BRILLO — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

Wire bonding of gold with conducting substrates such as aluminum is a widely used industrial technique. To understand the formation of the Al-Au interface, it is crucial to study the thermophysical properties of the binary Al-Au system in the liquid state. We measured the surface tension of liquid Al-Au alloys in a wide temperature and concentration range. The measurements have been performed containerlessly by electromagnetic levitation using the oscillating-drop technique. We compare the obtained experimental data with theoretical predictions from the Butler- and multilayer model.

MM 62: Topical session: X-ray and neutron scattering in materials science IV - High Energy Single Grain Diffraction

Time: Thursday 17:30–18:45

Location: BAR 205

Topical Talk MM 62.1 Thu 17:30 BAR 205
High Energy Single Grain Diffraction — ●ULRICH LIENERT — Deutsches Elektronen-Synchrotron, Hamburg, Germany

Over the last decade methodologies have been developed that enable the assignment of diffraction spots from multigrain diffraction patterns to individual grains. High energy synchrotron radiation has been employed for the investigation of polycrystalline bulk materials during thermo-mechanical processing. From an experimental point of view, the techniques can be classified according to the sample-to-detector distance which governs the real and reciprocal space coverage and resolutions. The grain boundary topology and orientation gradients have been evaluated from diffraction patterns observed in close proximity to the sample. Large area detectors positioned further away from the sample can still capture several complete diffraction rings and complete lattice strain tensors, center-of-mass grain positions, and volumes have been evaluated. Finally, area detectors have been placed very far behind the sample increasing reciprocal space resolution on cost of coverage. The formation and evolution of subgrain structure has been observed and radial peak profiles have been analyzed in terms of inter- and intra-subgrain strains. The basic principles will be reviewed and selected case studies will be presented.

MM 62.2 Thu 18:00 BAR 205

In situ investigation of phase transformations in friction stir welded steels using high-energy X-ray diffraction — ●MALTE BLANKENBURG, PETER STARON, ANDREAS STARK, TORBEN FISCHER, 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 influence important mechanical properties. An example is friction stir welding as a solid state joining process. Occurring non-equilibrium phases potentially reduce strength and toughness of a joint and are thus important to be studied. The intermediate stages of phase transformations in steels *during* the joining process can only be registered 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. Additionally, the phase transformations occurring in the steels used for friction stir welding were studied using a dilatometer in the synchrotron beam. With a fast area detector, time-resolved measurements with image rates up to 10 Hz were possible for both setups. The results on the phase content as a function of time obtained from the diffraction data in com-

bination with the dilatometer signal improves the understanding of the processes occurring during friction stir welding of the investigated steels.

MM 62.3 Thu 18:15 BAR 205

Diffusion brazing of γ -TiAl alloys: Investigations of the joint by electron microscopy and XRD — ●KATJA HAUSCHILDT, ANDREAS STARK, UWE LORENZ, NORBERT SCHELL, FLORIAN PYCZAK, and MARTIN MÜLLER — Helmholtz-Zentrum Geesthacht, Institut für Werkstofforschung, Geesthacht, Deutschland

Diffusion brazing is a potential method to repair parts made from TiAl-alloys. In this work the phase constituent and microstructure of the brazed zone for Ni- and Fe-based braze alloys are investigated. For this scanning electron microscopy including energy dispersive X-ray and electron backscattered diffraction were employed. In addition the distribution of phases and changes in lattice parameters in the brazed zone were identified by diffraction with high energy X-rays at the DESY synchrotron in Hamburg, Germany. The braze zone itself is composed of two to three transitional layers reassembling the phase constitution of a TiAl-alloy near the substrate and a microstructure similar to α/β -titanium alloys in the middle of the joint. Besides γ , α_2 and ω , additional phases, which are related to the presence of nickel or iron are also found. The brazed zone microstructure changes significantly during heat treatment, showing that the as-brazed state is far from thermodynamical equilibrium.

MM 62.4 Thu 18:30 BAR 205

Strain profile of magnetoelectric interfaces studied by X-ray diffraction methods — ●MADJID ABES¹, CHRISTIAN KOOPS¹, STJEPAN HRKAC¹, ADRIAN PETRARU², HERMANN KOHLSTEDT², BRIDGET MURPHY¹, and OLAF MAGNUSSEN¹ — ¹Institut für experimentelle und angewandte Physik, CAU Kiel, Germany — ²Institute of Electrical and Information Engineering Nanoelectronic, CAU Kiel, Germany

Understanding the coupling at the interface between piezoelectric (PE) and magnetostrictive (MS) components in magnetoelectric (ME) composites is essential for the optimization of these composites for sensor applications. A large ME response is only obtained if the lattice deformation induced by an external magnetic field in the MS material can be transferred efficiently to the PE material. To study the coupling at the buried ME composite interface we measured the lattice deformation in PbZr_{0.52}Ti_{0.48}O₃ (PZT)/CoFe₂O₄ (CFO) composites. These *in situ* grazing incidence [1] and high resolution X-ray diffraction were carried out in an applied magnetic or electric field. Surprisingly, the coupling between the components is not perfect for these epitaxial composite systems. We attribute to this to additional strain relax-

ation at grain boundaries reducing the strain transfer at the interface between the crystal lattices of both components. The authors thank the DFG SFB 855 for financial support.

[1] M. Abes et al., Appl. Phys. Lett., 102, 011601 (2013)

MM 63: Invited Talk (Hauptvortrag) Paris

Time: Friday 9:30–10:00

Location: BAR 205

Invited Talk MM 63.1 Fri 9:30 BAR 205
Water induced deformation of nanoporous materials —
 ●JOSEF KECKES — Institute of Physics, Montanuniversität Leoben, Austria

The actuation of solid materials by water is ubiquitous in everyday life, ranging for instance from humidity driven movement of plants to frost damage in roads and buildings. In many - although by far not all - scenarios, the basic mechanisms are governed by the adsorption, condensation, or freezing of water within narrow, often nanoscale pores within the material.

We use nanoporous silica-based materials with cylindrical pores on highly ordered hexagonal pore lattices as model systems to assess the

material deformation quantitatively. The nanoscale deformation can be monitored in-situ by measuring the pore lattice strain with X-ray diffraction as a function of pressure or temperature. The basic mechanisms of deformation due to condensation or freezing of water in the nanopores can be well understood by fundamental thermodynamic principles [1], although many details are still a matter of debate.

Beyond the understanding of the underlying mechanisms, we deposit nanoporous thin films on non-porous thin substrates. By this, simple humidity-actuated micro-devices based on bilayer structures can be fabricated and their performance can be studied.

[1] M. Erko, D. Wallacher, and O. Paris: Deformation mechanism of nanoporous materials upon water freezing and melting. Applied Physics Letters 101 (2012), 181905.

MM 64: Topical session: X-ray and neutron scattering in materials science V - X-ray Nanodiffraction Characterization of Inhomogeneous Structural and Mechanical Properties of Thin Films

Time: Friday 10:15–11:30

Location: BAR 205

Topical Talk MM 64.1 Fri 10:15 BAR 205
X-ray Nanodiffraction Characterization of Inhomogeneous Structural and Mechanical Properties of Thin Films —
 ●JOSEF KECKES — Department of Materials Physics, Montanuniversität Leoben, 8700 Leoben, Austria

Nanocrystalline and nanostructured thin films with grain size below 100nm exhibit typically inhomogeneous depth gradients of microstructure, strain and physical properties varying at the nano-scale. Currently, however, it is not trivial to reveal how these gradients relate to the macroscopic film behaviour. In this contribution, our recent results from position-resolved cross-sectional X-ray nanodiffraction studies of microstructure and strain in nanocrystalline films performed using monochromatic beams with diameters down to 50nm will be presented. On the examples of hard nitride coatings and metallic thin films, it will be demonstrated that the newly developed approaches can be used to analyse lateral- and thickness-dependent gradients of residual stress, crystallographic texture, phases and grain size with sub-micron resolution. Additionally, results from mechanical tests obtained from bending experiments on micro-cantilevers will be used to illustrate variability and anisotropy of mechanical properties in nanocrystalline coatings.

MM 64.2 Fri 10:45 BAR 205
Local strain and magnetization studies in single magneto-electric microcomposites — ●STJEPAN HRKAC¹, MADJID ABES¹, CHRISTIAN KOOPS¹, CHRISTINA KRYWKA^{2,3}, MARTIN MÜLLER^{1,2,3}, JEFFREY MCCORD⁴, SÖREN KAPS⁴, YOGENDRA MISHRA⁴, RAINER ADELUNG⁴, MANFRED BURGHAMMER⁵, OLAF MAGNUSSEN^{1,3}, and BRIDGET MURPHY^{1,3} — ¹Institute for Experimental and Applied Physics, University of Kiel, Germany — ²Institute of Materials Research, Helmholtz Zentrum Geesthacht, Germany — ³Ruprecht Haensel Laboratory, University of Kiel, Germany — ⁴Institute for Materials Science, University of Kiel, Germany — ⁵European Synchrotron Radiation Facility, Grenoble, France

Magnetolectric microcomposites are of interest for novel sensor application. We combine magneto-optic Kerr effect microscopy and nanofocus X-ray diffraction to map the local properties of ZnO micro-rods coated with an amorphous (Fe₉₀Co₁₀)₇₈Si₁₂B₁₀ layer. We follow the magnetic domain behavior and lattice deformation upon applying an external magnetic field. In addition to the expected field induced strain, we observe a local magnetic induced strain in the 10⁻⁵ range in the ZnO localized near the (Fe₉₀Co₁₀)₇₈Si₁₂B₁₀ /ZnO interface¹. Financial support via the German Science Foundation (DFG) SFB 855 is acknowledged.

¹S.B. Hrkac, M. Abes, C. T. Koops, C. Krywka, M. Müller, S. Kaps, R. Adelung, J. McCord, E. Lage, E. Quandt, O. M. Magnussen, and B. M. Murphy, Applied Physics Letters 103, 123111 (2013)

MM 64.3 Fri 11:00 BAR 205
Spider vibration sensor studied by X-ray scattering — ●MAXIM ERKO¹, FRIEDRICH G. BARTH², PETER FRATZL¹, and Yael POLITI¹ — ¹Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, D-14476 Potsdam — ²Universität Wien, Althanstrasse 14, A-1090 Wien

Vibration sensors of spiders are known for their remarkable sensitivity and specificity. They allow the detection and recognition of complex environmental signals with relatively little down-stream processing by the central nervous system. As a consequence of the material composition and the structural architecture of these cuticular strain detectors, environmental signals are not merely collected, but are preferentially filtered for those of biological relevance. We studied the relationship between structure and function by applying X-ray microbeam scanning diffraction to non-nervous cuticular structures transforming the mechanical stimulus on its way to the sensory cells which innervate the vibration sensor. Our results include quantitative maps of structural and compositional variations within the spider cuticle obtained from X-ray scattering signals at wide and small angles (WAXS,SAXS), respectively. The structural and compositional details of the organ are then related to the mechanical properties measured by scanning acoustic microscopy (SAM) and nanoindentation. The data allow us to propose new details about the signal filtering mechanism of the spider vibration sensor. Overall, this work unveils the working principle of material-based vibration-filters in nature and can provide valuable input for future applications in bio-inspired sensory technology.

MM 64.4 Fri 11:15 BAR 205
Investigation of the piezoelectric behaviour in bones on a micrometer length scale — ●D.C.F. WIELAND¹, D. KLUSS², E. MICK², C. KRYWKA¹, R. WILLUMET¹, and R. BADER² — ¹Helmholtz-Zentrum Geesthacht, Institut für Werkstofforschung, Max-Planck-Straße 1, 21502 Geesthacht, Germany — ²Universitätsmedizin Rostock, Orthopädische Klinik und Poliklinik, 18057 Rostock, Germany

Electromagnetic stimulation is a clinical treatment for improving bone healing e.g. in the femoral head in case of avascular necrosis. It is supposed to be based on the principle of a reciprocal piezoelectric effect in combination with piezoelectric properties of bone tissue. Therefore, we have investigated the structure of bone at different applied voltages

by means of micro diffraction at the nanofocus endstation of the P03., PETRA III, Germany. Slices of 150 μm thickness were cut from bovine trabecular bone and placed between two clamps designed to apply AC current on the sample. In order to extract the structure of the bone matrix at different positions with high resolution, the samples were scanned by a X-ray beam with the size of 1.5 μm . Each position was scanned over an array of 30 x 30 points within an area of 45 x 45 μm .

To determine the effect of voltage applied at the bone samples, the measurements were repeated at 0V, 5V and 10V. Our data hints that the hydroxyapatite crystals in the bone matrix, which amount 65% of the bone mass are subject to mechanical stress if the applied voltage is increased from 0 to 10V. Furthermore, this effect depends strongly on the orientation of collagen fibrils in the bone matrix. Other properties of the hydroxyapatite like the orientation of the crystals are unaffected.

MM 65: Topical session: X-ray and neutron scattering in materials science VI - Which orientations can we expect for elongated particles in self-confined systems?

Time: Friday 11:45–13:00

Location: BAR 205

Topical Talk

MM 65.1 Fri 11:45 BAR 205

Which orientations can we expect for elongated particles in self-confined systems? — •ULLA VAINIO¹, THEA SCHNOOR², JÜRGEN MARKMANN^{1,2}, KE WANG², KARL SCHULTE², JÖRG WEISSMÜLLER^{1,2}, ERICA LILLEODDEN¹, ANDREAS SCHREYER¹, and MARTIN MÜLLER¹ — ¹Helmholtz-Zentrum Geesthacht — ²Technische Universität Hamburg-Harburg

Many new novel composite materials aim at orienting particles within a matrix in a preferred direction. It is commonly known that orientations of crystals in metals have a strong impact on the mechanical properties of the metals, and we expect the same for nanocomposite materials in which the orientation of particles is to a large extent limited by self-confinement. An example of a self-confined system is a carbon nanotube forest with its long cylindrical nanotubes growing away from a substrate and creating a seemingly homogeneous array of nanotubes with vertical alignment. Here we show that this vertical alignment cannot be described accurately by any of the commonly used distribution functions such as Gaussian or Lorentzian. Instead, the orientation distribution was measured using small-angle X-ray scattering (SAXS) and was fitted best by the generalized normal distribution, which is an extension to the Gaussian and allows one more degree of freedom. In another example we use small-angle neutron scattering (SANS) to study the orientation of ligaments in a nanoporous gold composite. In this case we observe the nanostructure after applying compressive deformation and can follow the changes in the orientation of the ligaments.

MM 65.2 Fri 12:15 BAR 205

In-situ Synchrotron Studies of Colloidal Crystallisation and the Influence of the Nanocrystal Shape — •RAINER T. LECHNER¹, MAX BURIAN¹, CHRISTIAN PREHAL¹, MAKSYM YAREMA^{2,3}, HEINZ AMENITSCH⁴, WOLFGANG HEISS², and OSKAR PARIS¹ — ¹Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria — ²Institute of Semiconductor and Solid State Physics, JKU Linz, 4040 Linz, Austria — ³Integrated Systems Laboratory, ETH Zürich J87, 8092 Zurich, Switzerland — ⁴Institute of Inorganic Chemistry, TU Graz, 8010 Graz, Austria

Colloidal crystals using crystalline nanoparticles (NCs) as building blocks offer the opportunity for designing artificial solids [1] with tailored properties [2] used e.g. for nanoelectrodes [3]. The assembly of colloidal crystals is not only influenced by the NC-size, but also by the shape of the individual NC.

We studied by *in-situ* SAXS/WAXS the template free self-assembled colloidal crystallization by diffusion of a non-solvent into the colloidal dispersion [1]. The SAXS patterns of the NC ensembles were recorded below the NC-solvent/non-solvent interface at the SAXS beamline at ELETTRA. Hence, we can follow the crystallization process in short time steps as a function of the non-solvent concentration. Furthermore, we retrieved the mean particle shape of the NCs and could show the influence of the elliptical and faceted shape on the super-crystal structure.

[1] M. Yarema, *et al.*, ACS Nano 6, (2012) [2] D.V. Talapin, MRS Bull. 37, (2012) [3] M.Yarema, *et al.*, JACS 132, (2010)

MM 65.3 Fri 12:30 BAR 205

Stabilization of ZnO nanoparticles - a SAXS/SANS study — •TORBEN SCHINDLER, MARTIN SCHMIELE, TILO SCHMUTZLER, CHRISTINE BAUER, CAROLINE WEIS, and TOBIAS UNRUH — Work group nanomaterials characterization, Friedrich-Alexander University Erlangen Nuremberg, Staudtstr.3, 91058 Erlangen

Research on semiconductor nanoparticles (NPs) is of highest importance as the properties of the NPs can be adjusted due to the quantum size effect. For the integration in e.g. electronic devices or thin film solar cells, stable and well-defined NPs have to be designed, and knowledge about the nucleation and growth processes is crucial. The influence of surfactants is of highest importance as they have tremendous effects on the size and stability of the nanoparticles during preparation and storage, respectively.[1]

The influence of the stabilizer on the growth of zinc oxide nanoparticles was investigated using small angle neutron and X-ray scattering on the same sample. Only the use of both scattering techniques simultaneously allowed us to get detailed insight into the ripening process as SAXS is sensitive to the ZnO core and SANS to the stabilizing acetate shell. In this talk we will present the results from this combined approach to describe the ripening process not only by the changes of the size of the nanoparticles but also by the changes within the stabilizing layer which have a tremendous effect on the particle growth e.g. the stop of the ripening at a certain size.

[1]D. Segets et al., ACS Nano, 2011, 5 (6), 4658

MM 65.4 Fri 12:45 BAR 205

Ultrananocrystalline diamond films studied using GISAXS/GISANS — •HADWIG STERNSCHULTE¹, ISABELLA STAUDINGER¹, SEBASTIAN SIMETH¹, ALESSANDRO SEPE¹, CHRISTINE M. PAPADAKIS¹, JAN PERLICH², STEPHAN V. ROTH², JEAN-FRANCOIS MOULIN³, SLIMANE GHODBANE⁴, and DORIS STEINMÜLLER-NETHL⁴ — ¹TU München, Physik Department, Garching — ²DESY, Hamburg — ³Helmholtz-Zentrum Geesthacht, Garching — ⁴DiaCoating GmbH, Innsbruck, Austria

Ultrananocrystalline diamond (UNCD) films are characterised by their small grain size of less than 10nm and a smooth surface with RMS values down to 10nm independent of the film thickness. The diamond grains in round shapes embedded in an amorphous C:H matrix are randomly oriented. Usually, UNCD films are studied by transmission electron microscopy (TEM) to obtain information about the grain size and the distance of the grains in the matrix. One disadvantage of TEM on diamond is that a highly sophisticated preparation is needed. For the first time we analysed UNCD films with grazing-incidence small-angle X-ray [1] and neutron scattering (GISAXS/GISANS). For this study UNCD films were grown on Si substrates by a modified hot filament technique using a CH₄/H₂ gas mixture. Prior to the deposition, the substrates have been pre-treated by an ultrasonic bath with diluted diamond powder. By data modelling and simulation we analyzed in detail the GISAXS/GISANS maps. The results will be discussed in comparison with TEM images with respect to growth processes. [1] H. Sternschulte et al, Diamond Relat. Mater. 37 (2013) 68