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

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Overview of Invited Talks and Sessions

(Lecture rooms BAR 205, IFW A, IFW B, and IFW D; Poster P4)

Invited Talks

MM 1.1	Mon	9:30–10:00	BAR 205	**Liquid-liquid transition in metallic melts** — •Ralf Busch
MM 12.1	Mon	15:00–15:30	BAR 205	**From weakened chemical bonds to materials breakdown: An ab initio perspective** — •Mira Todorova
MM 23.1	Tue	9:30–10:00	BAR 205	**Integration of Grain Boundary Mechanics and Migration** — •David Srolovitz, Jian Han, Spencer Thomas, Vaclav Vitek
MM 45.1	Wed	15:00–15:30	BAR 205	**Diffusion in liquid metals and alloys** — •Florian Kargl
MM 53.1	Wed	18:30–19:00	BAR 205	**Small scale deformation behavior of high performance materials - Advanced mechanical testing meets high end microstructure characterization** — •Verena Maier-Kiener, Irmgard Weissensteiner, Benjamin Schuh, Anton Hohenwarter, Helmut Clemens
MM 54.1	Thu	9:30–10:00	BAR 205	**Revealing the mechanism of Z-phase formation in 12% Cr ferritic-martensitic steels** — •Daniel F. Urban, Christian Elsässer
MM 64.1	Thu	15:00–15:30	BAR 205	**Microstructural refinement, rate sensitivity and structural stability of Cu-X solid solutions after severe plastic deformation** — •Karsten Durst

Invited talks of the joint symposium SYLI

See SYLI for the full program of the symposium.

SYLI 1.1	Mon	9:30–10:00	HSZ 02	**Interfacial challenges in solid- state Li ion: some perspectives from theory** — •Alan Luntz, Saskia Stegmaier, Johannes Voss, Karsten Reuter
SYLI 1.2	Mon	10:00–10:30	HSZ 02	**Will solid electrolytes enable lithium metal anodes in solid state batteries?** — •Jürgen Janek, Dominik Weber, Wolfgang Zeier
SYLI 1.3	Mon	10:30–11:00	HSZ 02	**Hybrid Electrolytes for Solid-State Batteries** — •Hans-Dieter Wiemhöfer
SYLI 1.4	Mon	11:15–11:45	HSZ 02	**Neutron diffraction on solid-state battery materials** — •Helmut Ehrenberg, Anatoliy Senyshyn, Mykhailo Monchak, Sylvio Indris, Joachim Binder
SYLI 1.5	Mon	11:45–12:15	HSZ 02	**Sulfate-based Solid-State Batteries** — •Yuki Katoh

Invited talks of the joint symposium SYBM

See SYBM for the full program of the symposium.

SYBM 1.1	Tue	9:30–10:00	HSZ 02	**New twists in biological photonics: circular polarisation and beyond.** — •Pete Vukusic, Luke McDonald, Ewan Finlayson
SYBM 1.2	Tue	10:00–10:30	HSZ 02	**Bio-inspired materials and structures for technology and architecture** — •Thomas Speck
SYBM 1.3	Tue	10:30–11:00	HSZ 02	**Cellulose bio-inspired hierarchical structures** — •Silvia Vignolini

SYBM 1.4	Tue	11:15–11:45	HSZ 02	**Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing** — •Vladimir Tsukuruk
SYBM 1.5	Tue	11:45–12:15	HSZ 02	**3D laser nano-printing of rationally designed materials** — •Martin Wegener

Invited talks of the joint symposium SYNS

See SYNS for the full program of the symposium.

SYNS 1.1	Wed	15:00–15:30	HSZ 02	**The Limits to Lithography: How Electron-Beams Interact with Materials at the Smallest Length Scales** — •Karl K. Berggren
SYNS 1.2	Wed	15:30–16:00	HSZ 02	**High precision fabrication for light management at nanoscale** — •Saulius Juodkazis, Armandas Balcytis
SYNS 1.3	Wed	16:00–16:30	HSZ 02	**Directed self-assembly of performance materials** — •Paul Nealey
SYNS 1.4	Wed	16:45–17:15	HSZ 02	**Nanometer accurate topography patterning using thermal Scanning Probe Lithography** — •Armin W. Knoll
SYNS 1.5	Wed	17:15–17:45	HSZ 02	**High resolution 3D nanoimprint lithography** — •Hartmut Hillmer

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	10:30–11:00	HSZ 02	**Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations** — •Weitao Yang
SYES 1.2	Fri	11:00–11:30	HSZ 02	**Multi-reference density functional theory** — •Andreas Savin
SYES 1.3	Fri	11:30–12:00	HSZ 02	**Density functionals from machine learning** — •Kieron Burke
SYES 1.4	Fri	12:00–12:30	HSZ 02	**Taming Memory-Dependence in Time-Dependent Density Functional Theory** — •Neepa Maitra
SYES 1.5	Fri	12:30–13:00	HSZ 02	**Quantum Embedding Theories** — •Fred Manby

Sessions

MM 1.1–1.1	Mon	9:30–10:00	BAR 205	**Invited talk Busch**
MM 2.1–2.5	Mon	9:30–12:15	HSZ 02	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Invited talks**
MM 3.1–3.4	Mon	10:15–11:30	BAR 205	**Topical Session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Segregation and Embrittlement I**
MM 4.1–4.4	Mon	10:15–11:30	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses I - Structural Transitions**
MM 5.1–5.5	Mon	10:15–11:30	IFW B	**Computational Materials Modelling: Materials at finite temperatures**
MM 6.1–6.4	Mon	10:15–11:15	IFW D	**Structural Materials**
MM 7.1–7.10	Mon	10:30–13:00	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I**
MM 8.1–8.6	Mon	11:45–13:15	BAR 205	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Segregation and Embrittlement II**
MM 9.1–9.6	Mon	11:45–13:15	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses II - Undercooled Melts**
MM 10.1–10.6	Mon	11:45–13:15	IFW B	**Computational Materials Modelling - Accelerated Approaches**
MM 11.1–11.7	Mon	11:45–13:30	IFW D	**Biomaterials**
MM 12.1–12.1	Mon	15:00–15:30	BAR 205	**Invited talk Todorova**
MM 13.1–13.12	Mon	15:00–18:15	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II**

MM 14.1–14.6	Mon	15:45–17:15	BAR 205	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Electro- and mechno-chemical coupling**
MM 15.1–15.4	Mon	15:45–16:45	IFW A	**Symposium SYLI: Interfacial Challenges in Solid-State Li Ion Batteries - Interface-dominated behaviour**
MM 16.1–16.4	Mon	15:45–16:45	IFW B	**Computational Materials Modelling - Novel Materials**
MM 17.1–17.5	Mon	15:45–17:00	IFW D	**Functional Materials I**
MM 18.1–18.4	Mon	17:30–18:45	BAR 205	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Experimental Characterization**
MM 19.1–19.3	Mon	17:15–18:00	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - sulphate- and phosphate-based electrolytes**
MM 20.1–20.5	Mon	17:00–18:15	IFW B	**Computational Materials Modelling - Defect structure and formation**
MM 21.1–21.6	Mon	17:15–18:45	IFW D	**Functional Materials II**
MM 22.1–22.41	Mon	19:00–20:00	P4	**Poster session I**
MM 23.1–23.1	Tue	9:30–10:00	BAR 205	**Invited talk Srolovitz**
MM 24.1–24.5	Tue	9:30–12:15	HSZ 02	**Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs**
MM 25.1–25.4	Tue	10:15–11:30	BAR 205	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and Deformation I**
MM 26.1–26.5	Tue	10:15–11:30	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - NMR studies**
MM 27.1–27.4	Tue	10:15–11:15	IFW B	**Computational Materials Modelling - Electronic structure approaches**
MM 28.1–28.6	Tue	10:15–11:45	IFW D	**Transport I - atomic transport**
MM 29.1–29.9	Tue	10:30–13:00	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III**
MM 30.1–30.5	Tue	11:45–13:00	BAR 205	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and Deformation II**
MM 31.1–31.4	Tue	11:45–12:45	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Structure - property relationships I**
MM 32.1–32.6	Tue	11:45–13:15	IFW B	**Microstructure and Phase Transformations - detection methods**
MM 33.1–33.4	Tue	12:00–13:00	IFW D	**Transport II - charge transport**
MM 34.1–34.42	Tue	18:30–20:30	P4	**Poster session II**
MM 35.1–35.12	Tue	18:30–20:30	P2-OG4	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond**
MM 36.1–36.1	Wed	9:30–10:00	BAR 205	**Invited talk Curtin**
MM 37.1–37.5	Wed	10:15–11:45	BAR 205	**Topical session: Data driven materials design - defect engineering**
MM 38.1–38.5	Wed	10:15–11:30	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - defects, structure and thermodynamics**
MM 39.1–39.4	Wed	10:15–11:15	IFW B	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and deformation III**
MM 40.1–40.4	Wed	10:15–11:15	IFW D	**Transport III - thermal transport**
MM 41.1–41.9	Wed	10:30–13:00	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV**
MM 42.1–42.4	Wed	12:00–13:15	BAR 205	**Topical session: Data driven materials design - high throughput**
MM 43.1–43.4	Wed	11:45–12:45	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - hybrid and structured electrolytes**
MM 44.1–44.6	Wed	11:30–13:15	IFW B	**Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Nanoporous materials**
MM 45.1–45.1	Wed	15:00–15:30	BAR 205	**Invited talk Kargl**
MM 46.1–46.13	Wed	15:00–18:15	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V**

MM 47.1–47.4	Wed	15:45–17:00	BAR 205	**Topical session: Data driven materials design - ab initio materials design**
MM 48.1–48.5	Wed	15:45–17:15	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses III - plasticity and hetererogeneities**
MM 49.1–49.4	Wed	15:45–16:45	IFW B	**Microstructure and Phase Transformations - shape memory alloys**
MM 50.1–50.4	Wed	15:45–16:45	IFW D	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Structure - property relationships II**
MM 51.1–51.3	Wed	17:15–18:00	BAR 205	**Topical session: Data driven materials design - databases**
MM 52.1–52.4	Wed	17:00–18:00	IFW B	**Microstructure and Phase Transformations - phase stability**
MM 53.1–53.1	Wed	18:30–19:00	BAR 205	**Invited talk Maier-Kiener**
MM 54.1–54.1	Thu	9:30–10:00	BAR 205	**Invited talk Urban**
MM 55.1–55.6	Thu	10:15–11:45	BAR 205	**Topical session: Data driven materials design - structure maps**
MM 56.1–56.4	Thu	10:15–11:30	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses - kinetic transitions**
MM 57.1–57.4	Thu	10:15–11:15	IFW B	**Microstructure and Phase Transformations - transformation kinetics**
MM 58.1–58.6	Thu	10:15–11:45	IFW D	**Nanomaterials I**
MM 59.1–59.13	Thu	10:30–13:45	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI**
MM 60.1–60.5	Thu	12:00–13:15	BAR 205	**Topical session: Data driven materials design - machine learning**
MM 61.1–61.5	Thu	11:45–13:15	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses V - dynamical response**
MM 62.1–62.5	Thu	11:45–13:00	IFW B	**Microstructure and Phase Transformations - nucleation kinetics and pressure effects**
MM 63.1–63.6	Thu	12:00–13:30	IFW D	**Nanomaterials II**
MM 64.1–64.1	Thu	15:00–15:30	BAR 205	**Invited talk Durst**
MM 65.1–65.3	Thu	15:45–16:30	BAR 205	**Topical session: Data driven materials design - uncertainity approaches**
MM 66.1–66.5	Thu	15:45–17:15	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses VI - mechanical properties**
MM 67.1–67.4	Thu	15:45–16:45	IFW D	**Mechanical Properties I**
MM 68.1–68.9	Thu	16:00–18:30	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII**
MM 69.1–69.6	Thu	17:30–19:00	IFW A	**Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses VII - thermodynamics and structure**
MM 70.1–70.5	Thu	17:00–18:15	IFW D	**Mechanical Properties II**
MM 71.1–71.5	Fri	10:30–13:00	HSZ 02	**Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond**

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:30–20:30 BAR 205

MM 1: Invited talk Busch

Time: Monday 9:30–10:00 Location: BAR 205

Invited Talk MM 1.1 Mon 9:30 BAR 205

Liquid-liquid transition in metallic melts — •Ralf Busch — Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany

Recently polymorphic transitions within the liquid state termed polyamorphisms have been observed or proposed. In this contribution experiments on kinetics, thermodynamics and structure of molten bulk metallic glass forming alloys in the equilibrium state as well as in the undercooled state are presented

In the case of Zr41.2Ti13.8 Cu12.5Ni10.0Be22.5 (Vit1) we observe sudden changes of viscosity of 2 orders of magnitude [1] that are associated with a latent heat in the absence of crystalline reflexes under synchrotron radiation. These effects are observed upon cooling and heating and exhibit a pronounced hysteresis. The results suggest that the Vit 1 liquid alloy undergoes a weak first order phase transformation likely from a short range ordered fragile state at high temperatures to a medium range ordered strong state at low temperatures [2]. This behavior is also clearly observed in Zr58.5Cu15.6Ni12.8Al10.3Nb2.8 (Vit106a) [3]. The change in fragility can be quantitatively linked to structural changes that are observed by synchrotron radiation [4].

[1]*C. Way, P. Wadhwa, and R. Busch, Acta Materialia 55 (2007) 2977*2983. [2]*S. Wei et al. Nat Comm. 4 (2013) 2083. [3]*M. Stolpe et al., Phys. Rev. B 93, 014201. [4]*S. Wei et al., Appl. Phys. Lett. 106 (2015) 181901.

MM 2: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Invited talks

Time: Monday 9:30–12:15 Location: HSZ 02

Invited Talk MM 2.1 Mon 9:30 HSZ 02

Interfacial challenges in solid- state Li ion: some perspectives from theory — •Alan Luntz[1], Saskia Stegmaier[1], Johannes Voss[1], and Karsten Reuter[2] — [1]Stanford University, Stanford, CA, USA — [2]Technical University of Munich, Munich, Germany

Unfortunately, interfacial challenges severely limit power and cycle life in all solid- state Li ion batteries. We use theory to investigate some of the origins of these limitations with both continuum theory and DFT. The obvious ones are electrochemical stability of the electrolyte at the anode/cathode interfaces and mechanical issues relating to maintaining interfacial contact during cycling while inhibiting Li dendrite growth. We are especially trying to understand if any fundamental limitations exist from the structures of the double layers that form at the solid electrolyte- electrode or other interfaces in the solid-state stack. These can be quite different than in conventional liquid Li ion batteries. We use Li3OCl as a prototypical Li ion superionic conductor and discuss its properties and discuss its interface with model electrode interfaces.

Invited Talk MM 2.2 Mon 10:00 HSZ 02

Will solid electrolytes enable lithium metal anodes in solid state batteries? — •Jürgen Janek, Dominik Weber, and Wolfgang Zeier — Institut für Physikalische Chemie, Justus Liebig-Universität, Gießen, Germany

In order to achieve solid state lithium batteries with higher energy densities [1], lithium metal anodes are one of the primary options. However, reversible and morphologically stable plating of thick lithium metal films is difficult, as void formation and dendrite growth may occur - leading to impedance growth and/or short-circuits. Ceramic electrolytes are considered as a potential solution to this problem. In this lecture the interface between solid electrolytes and lithium metal anodes will be discussed in depth, and the occurrence of both thermodynamic and kinetic instabilities will be highlighted. In particular, the existence of SEI (”solid electrolyte interphases”), forming between lithium metal and the solid electrolyte, will be demonstrated for a number of solid electrolytes. It will also be shown that the growth of these SEI layers follows a typical square-root law-type behavior in SEI formation in liquid electrolytes.

[1] J. Janek and W. Zeier, Nat. Energy 1 (2016) 16141

Invited Talk MM 2.3 Mon 10:30 HSZ 02

Hybrid Electrolytes for Solid-State Batteries — •Hans-Dieter Wiemhöfer — Inst. Inorganic & Analyt. Chem., WWU Münster — Helmholtz-Institute Münster

Rechargeable lithium batteries with largely increased energy and power densities are a primary goal at present world wide. At the same time, enhanced safety concerns cause the need to replace current liquid electrolytes by new high performance electrolytes combining higher mechanical, thermal and electrochemical stability. Finally, this leads to the development of hybrid electrolytes. The primary idea is to construct electrolytes fulfilling a multitude of requirements based on a combination of components and phases, often coupled with approaches to achieve stable meso or micro porous networks down to chemically designed nanostructures. Starting from ion conducting inorganic solids and glasses, the combination with polymers and salt-in-polymer systems opens a wide range for possibilities for chemical design, tailoring and fine tuning of electrolyte properties of such hybrid systems. The concept will be illustrated with a number of examples, for instance, self organized block-copolymer networks acting as porous containers for fast ion conducting channels. Future all solid state batteries are expected to profit from hybrid concepts as well. For instance, volume changes during charging/discharging of active electrodes need an elastic polymer network acting as a glue and stabilizing a good contact and charge transfer kinetics of solid electrolyte/solid electrode interfaces.

15 min. break

Invited Talk MM 2.4 Mon 11:15 HSZ 02

Neutron diffraction on solid-state battery materials — •Helmut Ehrenberg[1], Anatoliy Senyshyn[2], Mykhailo Monchak[1], Sylvio Indris[1], and Joachim Binder[1] — [1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM) — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitaet Muenchen, Garching, Germany

Solid-state batteries are a promising approach to safer electrochemical energy storage and higher energy densities. Bottle necks are interface reactions and transport limitations in the solids. Advanced and optimized materials must provide dedicated properties, for example a good Li-ion conductivity for sufficiently high current densities and only small volume changes to preserve mechanical integrity. Neutron diffraction offers unique features to elucidate the underlying structure-property relationships, which determine the resulting performance parameters on cell level. Selected examples are shown, which demonstrate the capabilities of neutron diffraction to reveal Li-ion diffusion pathways as in the $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) superionic conductor, Li occupation numbers at intermediate states of charge as for $LiCoPO_4$ or a comparison of volume changes between commercial and alternative zero-strain electrode materials. The capabilities of solid-state batteries are discussed.

Invited Talk MM 2.5 Mon 11:45 HSZ 02

Sulfate-based Solid-State Batteries — •Yuki Katoh — Toyota Motor Europe NV/SA, Hoge Wei 33, Zaventem, Belgium

Large-scale batteries are in high demand for applications such as plug-in electric hybrid or electric vehicles, and smart electric power grids. The all-solid-state battery is the most promising candidate for future battery systems, due to the high energy density obtaining by direct-series-stacking of the battery cells. However, the poor electrochemical characteristics of the all-solid-state battery, due to higher cell-resistivity than conventional liquid electrolyte batteries, still remain as an unsolved issue. We will demonstrate an all-solid-state battery with extremely high power performance that employs the superionic conductors having the Li10GeP2S12-type crystal structure. The battery can operate over a wide temperature range with extremely high current drains of 3 mAcm-2 (-30 C), 100 mAcm-2 (25 C), and 1000 mAcm-2 (100 C). Careful electrochemical examination of the all-solid-state battery with the same battery configuration as a liquid electrolyte system revealed that the rate characteristics are simply dependent on the difference in state of electrolyte. The vert high power characteristics of solid state battery comes from intrinsic ion transportation mechanism of solid electrolyte.

MM 3: Topical Session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Segregation and Embrittlement I

Time: Monday 10:15–11:30 Location: BAR 205

Topical Talk MM 3.1 Mon 10:15 BAR 205

Tensile strength in ab initio simulations: stability of models with planar defects — •Petr Šesták[1,2], Miroslav Černý[1,2], Monika Všianská[1,2], and Mojmír Šob[1,2,3] — [1]Institute of Physics of Mater., Academy of Sci. of CZ, Brno, CZ — [2]Central European Institute of Technology, Brno, CZ — [3]Faculty of Science, Masaryk University, Brno, CZ

Ab initio simulations represent an efficient way how to study material properties in those cases where experimental methods are too expensive or impossible to use. However, periodic boundary conditions employed in such simulations impose severe limitations to the size of the simulation cell that can contain just a few hundred atoms at the most. Correct design of appropriate computational cells and simulation models is then a crucial issue in applications of ab initio approaches in simulations of defects.

Here we provide a critical comparison of several models often used for determination of the tensile strength of crystalline systems with planar defects (such as the $\Sigma3$ (111), $\Sigma5$ (210), $\Sigma5$ (310) and $\Sigma11$ (311) grain boundaries in fcc nickel) and interfaces in selected composites. Special attention is paid to differences in predictions of individual models and to their sensitivity to the size of the simulation cell (i.e. to different density of defects).

MM 3.2 Mon 10:45 BAR 205

Engineering the chemistry of grain boundaries in Mo-Hf alloys — •Daniel Scheiber[1], Katharina Leitner[2], Reinhard Pippan[3], Peter Puschnig[4], and Lorenz Romaner[1] — [1]Materials Center Leoben, Austria — [2]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Austria — [3]University of Graz, Institute of Physics, Austria — [4]Erich Schmid Institut of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Molybdenum alloys are known for their outstanding material properties like low thermal expansion coefficients and high strength at elevated temperatures. However, many Mo alloys are prone to brittle intergranular fracture at room temperature, which is attributed to low grain boundary (GB) cohesion. GB engineering searches for ways to counteract the low GB cohesion, e.g. by alloying with elements that segregate to the GB and enhance GB cohesion. In this study, Mo samples with different Hf contents are investigated, which exhibit a change from intergranular fracture to transgranular fracture with increasing Hf content. To reveal the underlying effects of this change in fracture mode, different experimental and theoretical methods are applied. A detailed atom probe tomography (APT) study shows the change in GB chemistry for the alloys and clarifies that not Hf, but rather segregated B and C atoms lead to the increase in GB cohesion. Subsequent ab-initio simulations of a GB observed in APT allows for comparison of the GB chemistry with experiment. With the agreement at hand, the simulations explain the change in GB chemistry and provide recommendations for Mo alloys with reduced intergranular fracture.

MM 3.3 Mon 11:00 BAR 205

Influence of hydrogen on grain boundary cohesion in nickel — •Matous Mrovec[1,2], Davide Di Stefano[2], Benedikt Ziebarth[2], and Christian Elsässer[2] — [1]ICAMS, Ruhr-Univeritát Bochum — [2]Fraunhofer IWM, Freiburg

The presence of hydrogen in metals often leads to marked lowering of their ductility, fracture strength and fracture toughness - a phenomenon commonly known as hydrogen embrittlement (HE). One of possible HE mechanisms is related to segregation of hydrogen at grain boundaries (GBs) that weakens the GB strength and results in easier intergranular decohesion. It has been observed that the susceptibility to hydrogen-induced intergranular embrittlement varies for different microstructures and hydrogen concentrations. However, quantitative knowledge of key quantities such as hydrogen binding energies at various GBs or critical hydrogen concentrations for fracture is still limited.

In this theoretical study, we explore the interaction of H with several grain boundaries in Ni at the atomic scale using first principles calculations based on density functional theory (DFT). We calculate H diffusion barriers and segregation energies in the vicinity of the GBs and relate these quantities to the geometrical characteristics of structural units composing the GBs. In addition, we also investigate the influence of H concentration on the cohesive behavior of the investigated GBs and compare the theoretical predictions with existing experimental results.

MM 3.4 Mon 11:15 BAR 205

Effects of alloying elements on H embrittlement of C segregated grain boundaries in bcc Fe — •Aparna P. A. Subramanyam, Abril Azocar Guzman, Xiang Huang, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr University-Bochum, Bochum, Germany

The cohesion of grain boundaries (GBs) is dependent on their chemical composition and structure and greatly influences the mechanical properties of the material. It is well known that H prefers segregating to the GBs (and other defects). H enhanced decohesion is one important mechanism of H embrittlement. Therefore it is necessary to understand the effects of alloying additions on the segregation behaviour of H and on the embrittling mechanism.

The embrittling effects of H in the presence of alloying elements Mn, Cr, V and C at the $\Sigma5(310)[001]36.9^\circ$ STGB and for selected cases, $\Sigma3(112)[1\bar{1}0]$ STGB in α-Fe was investigated by performing spin polarized DFT calculations with respect to a varying number of alloying elements and H atoms at different segregation sites of the GBs. The impact of co-segregation of Mn-C-H, Cr-C-H, V-C-H on GB energy, work of separation and theoretical strength has been studied. Uni-axial tensile tests were performed perpendicular to the GB and theoretical strength was determined from energy-displacement data fitted using the universal binding energy relationship. The thermodynamic model of Rice and Wang was used to determine the (cohesion enhancing or weakening) nature of the segregated elements. Based on our results, we discuss the alloying strategy to prevent H embrittlement of GBs.

MM 4: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses I - Structural Transitions

Time: Monday 10:15–11:30 Location: IFW A

Topical Talk MM 4.1 Mon 10:15 IFW A

Structural transition upon vitrification in viscous metallic liquids — •Andreas Meyer — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Köln

We investigate vitrification of bulk-glass forming Zr-Ni-Cu-Ti-Be and Zr-Cu-Ni-Al-Nb liquids from the equilibrium melt to the glass transition in-situ with container-less processing. Electrostatic levitation gives access to the measurement of temperature, density and in combination with X-ray diffraction to the total structure factor. Free radiation cooling of the sample allows the measurement of the specific heat over constant emissivity of the sample, which exhibits a pronounced peak in the deeply undecooled melt. This comes along with a change in the temperature dependence of the position of the first sharp diffraction peak, whereas the thermal expansion of the sample does not exhibit a detectable change over the entire temperature range. In addition, indirect information on the specific heat of the sample is obtained by precise measurement of the required heating laser power. All measurements reveal a consistent onset of changes in the total structure factor and the specific heat with no detectable cooling rate dependence. Results are discussed in the context of liquid-liquid phase transitions and the mode coupling theory of the liquid to glass transition.

MM 4.2 Mon 10:45 IFW A

Identifying structural changes in the medium range order of metallic glasses by Fluctuation Electron Microscopy (FEM) — •Dominik Tönnies, Lin Tian, and Cynthia A. Volkert — Institute of Materials Physics, University of Göttingen, Germany

The structural heterogeneity of a metallic glass (MG) is known to have tremendous impact on many important properties of the system, such as the mechanical performance and the formation of shear bands. While it is commonly understood how to *qualitatively* alter the structure by thermal and mechanical treatments, it is still extremely difficult to *precisely quantify* the subtle changes in the real-space order induced by structural alterations. For the characterization of medium range order (MRO) of an amorphous system, the method of Fluctuation Electron Microscopy (FEM) has been found useful in the past. In this method, very small volumes of the MG structure are probed by an electron beam in the Transmission Electron Microscope (TEM). Information about changes in the MRO is subsequently inferred from pixel variances of diffraction patterns taken at many different sample sites. We have used this technique to characterize the structure of a $Pd_{77.5}Cu_6Si_{16.5}$ MG at different structural states induced by thermal annealing, cooling to cryogenic temperatures, and mechanical rejuvenation. The results will be compared with nanoindentation pop-in studies to understand the influence of structure on the onset of mechanical deformation.

MM 4.3 Mon 11:00 IFW A

Signature of the atomic structure in the thermophysical properties of flint and metallic glasses — •Simon Hechler[1], Isabella Gallino[1], Moritz Stolpe[1], Frank-Thomas Lentes[2], and Ralf Busch[1] — [1]University of the Saarland, 66123 Saarbrücken, Germany — [2]Schott AG, 55122 Mainz, Germany

Flint glasses are silicates with large lead oxide content. From the experimental point of view, these glasses are the ideal network glass formers to compare metallic glasses with as they exhibit comparable glass transition temperatures. Metallic glasses are multicomponent atomic glass formers. The structure of these two types of glasses is completely different. Flint glasses build networks by connecting silicon and lead over bridging oxygen atoms with covalent or even ionic bondings. Metallic glasses have non-directional metallic bonds and a less ordered clustered structure. The differences in the structure of these materials manifests in their thermophysical properties like the specific heat capacity and viscosity. For understanding the structure property relationship in glasses, three flint glasses with different lead content are investigated in terms of specific heat capacity and viscosity and compared to metallic glass formers.

MM 4.4 Mon 11:15 IFW A

Structural reordering in CuZr-based metallic glass via short term sub-Tg annealing — •Baran Sarac[1], Andrea Bernasconi[2], Jonathan Wright[3], Mihai Stoica[4], and Jürgen Eckert[1] — [1]Erich Schmid Institute of Materials Science, OeAW, Leoben, Austria — [2]Dept. of Chemistry University of Pavia, Pavia, Italy — [3]ESRF-The European Synchrotron, Grenoble, France — [4]ETH Zurich, Department of Materials, Zürich, Switzerland

This work highlights the structural reordering and nanocrystallization behaviour of a recently in-house developed Cu46Zr44Al8Hf2 bulk metallic glass upon short term sub-glass transition annealing. This special type of heat treatment process generated work hardening confirmed by three-point bend tests. Structural reordering is investigated via high energy synchrotron X-ray diffraction ($\lambda = 0.01239$ nm), and compare the results with the structural modifications obtained from transmission electron microscopy (TEM) and conventional X-ray diffraction with Co Kα radiation ($\lambda = 0.01789$ nm). 2D diffraction image displays remarkable diffraction spots from different phases, where the total structure factor S(Q) tends to decrease upon heat treatment. Real-space pair distribution function (PDF) analysis reveals the peak shifts and thereby, changes within the short- to medium-range ordering. The changes in the average coordination number and distances between atom pairs upon annealing is studied from the first coordination shell of the radial distribution function (RDF), where the Gaussian fitting provided us the dominant atom pairs within the as-cast state and the annealed metallic glass.

MM 5: Computational Materials Modelling: Materials at finite temperatures

Time: Monday 10:15–11:30 Location: IFW B

MM 5.1 Mon 10:15 IFW B

Accurate electronic free energies of the transition metals at high temperatures — •Xi Zhang[1], Blazej Grabowski[1], Fritz Körmann[1,2], Christoph Freysoldt[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany — [2]Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, Netherlands

Free energies of bulk materials are nowadays routinely computed by density functional theory. In particular for metals, electronic excitations can significantly contribute to the free energy. Neglecting non-adiabatic contributions, electronic free energies can be obtained at relatively low computational cost, e.g., from the electronic density of states (DOS) at $T = 0$ K or by utilizing the Sommerfeld approximation. However, the actual error introduced by such approximations and the electron-phonon coupling effect at elevated temperatures is rarely known, even though it could affect, e.g., theoretical phase stability predictions. In order to clarify these issues we have computed the electronic free energies for all 3*d*, 4*d*, and 5*d* transition elements in the bcc, fcc, and hcp structures. For selected elements we have performed *ab initio* molecular dynamic simulations to investigate the electron-phonon coupling effect. We provide an analysis of the observed chemical trends in terms of the electronic DOS and the canonical *d* band model. The error in the approximate methods as well as the specific validity ranges for their application are clarified. The electronic heat capacities of all investigated elements as well as the error analysis within the Sommerfeld model are also presented.

MM 5.2 Mon 10:30 IFW B

Sampling of the magnetic structure in bcc and fcc iron using bond-order potentials — •Martin Staadt[1], Jutta Rogal[1], Tilmann Hickel[2], Thomas Hammerschmidt[1], Jörg Neugebauer[2], and Ralf Drautz[1] — [1]Interdisciplinary Centre for

Advanced Materials Simulation, Ruhr-Universität Bochum, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The phase transition between bcc and fcc iron is well known for its importance in manufacturing and processing of steels. We use a Metropolis Monte Carlo sampling algorithm with a non-collinear magnetic bond-order potential to sample the magnetic structure of bcc and fcc iron at various temperatures. Our approach includes simultaneous sampling of atomic and magnetic degrees of freedom and therefore implicitly accounts for magnon-phonon coupling. We show that we achieve a sensible description of the magnetic phase transformation and discuss the structural first order bcc-fcc phase transition. We will also present inital work on the prediction of temperature dependent local magnetic properties at grain boundaries and bcc-fcc interfaces.

MM 5.3 Mon 10:45 IFW B

Hot carriers Relaxation Dynamics in Hybrid Perovskites — •Mohamed El-Amine Madjet — Qatar Environment and Energy Research Institute(QEERI), Hamad bin Khalifa University(HBKU), Doha, Qatar

Hybrid organic-inorganic perovskites, such as methylammonium lead iodide CH3NH3PbI3, have attracted a lot of attention as promising new absorber materials for solar energy. Recently, perovskite-based solar cells reported a conversion efficiency of more than 22%. However, many fundamental processes related to the photophysics of these materials remain not fully understood. The excitation of electrons from the valence band to conduction band results in the formation of hot electrons and holes. Right after this photo-excitation an ultrafast thermalization of the hot carriers takes place driven by electron-phonon interaction.

A mixed quantum-classical approach based on trajectory surface hopping is used in order to investigate the process of non-radiative carrier relaxation in perovskite. Results will be presented for different perovskite materials depending on their structures and compositions and will discuss ways how the thermalization time could be enhanced.

MM 5.4 Mon 11:00 IFW B

Dynamical Material Parameters in Molecular Dynamics Simulations of Laser Ablation — •Johannes Roth[1], Eugen Eisfeld[1], Stefan Scharring[2], Marco Patrizio[3], Hans-Albert Eckel[2], and Mikhail Povarnitsyn[4] — [1]FMQ, Universit\"at Stuttgart — [2]DLR Stuttgart — [3]TU Darmstadt — [4]JIHT, RAS Moskau

Laser ablation is studied with classical molecular dynamics simulations. The interaction of the laser with the free electrons in the metallic material is modeled with a two-temperature model with separate temperatures for the electrons and the atoms. The properties of the electrons, heat capacity and conductivity and the electron-phonon-coupling as well as the reflectivity of the laser are model as constants for femto-second pulses since they do not change during the short time of interaction. This assumption is no longer valid for pico- and nanosecond pulses. We have implemented wide-range models for the electronic parameters similar to the work of Povarnitsyn [1] which describe the transition from the metal to the plasma state. The reflectivity is calculated dynamically with the Fresnel equations and the absorption with the help of the Helmholtz equations instead of the simple Lambert-Beer law. The improved results are compared to simulations carried out by hydrodynamic simulations.

[1] Povarnitsyn et al., Appl. Surf. Sci \textbf{258} (2012) 9480.

MM 5.5 Mon 11:15 IFW B

Investigation of low temperature features in the heat capacity of metals — •Ankit Gupta[1], Bengü Tas Kavakbasi[2], Biswanath Dutta[1], Blazej Grabowski[1], Tilmann Hickel[1], Sergiy Divinski[2], Gerhard Wilde[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Inst. of Materials Physics, Univ. of Münster, Münster, Germany

Heat capacities are often used to assess the predictive capability of computational thermodynamics, since they are experimentally directly accessible and as second derivatives very sensitive to energy changes. Finite-temperature first-principles calculations have accurately described the heat capacity of various material systems up to the melting point. In contrast, their assessment for the competition and coupling between the electronic and vibrational excitation mechanisms in the low-temperature regime is still in its infancy.

In this work, we explore this competition and coupling in the heat capacity C_p below 20 K for the example of Al and $\mathrm{Al_3Sc}$. In order to enhance the sensitivity with respect to low temperature features, we analyze C_p/T^n for $n = 0, \ldots, 3$. We show that, density functional theory successfully resolves all the features observed in the recent experimental calorimetric data, including the low-temperature limit and localization effects in the heat capacity. The relevance of peaks in the phonon density-of-states beyond the Debye level and non-adiabatic electron-phonon coupling phenomena are evaluated. All mechanisms are found to be described accurately at the level of semi-local exchange-correlation functionals.

MM 6: Structural Materials

Time: Monday 10:15–11:15 Location: IFW D

MM 6.1 Mon 10:15 IFW D

Ordering and thermodynamic properties of refractory NbMoTaW alloy from first-principles — •Fritz Körmann[1], Andrei V. Ruban[2,3], and Marcel H.F. Sluiter[1] — [1]Materials Science and Engineering, Delft University of Technology, Delft, Netherlands. — [2]Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden. — [3]Materials Center Leoben, Leoben, Austria.

Some refractory high entropy alloys (HEA) exhibit high-temperature mechanical properties that exceed modern Ni-based super alloys. However, little is known about their fundamental physical properties such as, e.g. ground states, degree of chemical ordering at elevated temperatures or thermodynamic properties. We present a combined first-principles and Monte Carlo (MC) study to investigate ordering at elevated temperatures in the prototype BCC HEA NbMoTaW [1]. Chemical interactions have been computed from first-principles by means of the coherent potential approximation in combination with the screened generalized perturbation method. Local relaxations have been considered by explicit super cell calculations. Surprisingly, the NbMoTaW solid-solution at elevated temperatures does not originate from the small magnitude but rather from the highly frustrated long-ranged nature of the chemical interactions. The role of the chemical interactions and ordering on thermodynamic properties is examined in detail [2]. [1] F. Körmann, A.V. Ruban, M.H.F. Sluiter, Materials Research Letters (2016), DOI 0.1080/21663831.2016.1198837 [2] F. Körmann, M.H.F. Sluiter, Entropy 18, 403 (2016).

MM 6.2 Mon 10:30 IFW D

Micromechanical behavior in dependence of the microstructure of nickel-based superalloys — •Robert Lawitzki[1], Jonas Woste[2], Michael Hofmann[3], Christian Krempaszky[2], Di Wang[4], Guido Schmitz[1], and Julia Wagner[1] — [1]Universität Stuttgart, Institut für Materialwissenschaft, 70569 Stuttgart — [2]TU München, Lehrstuhl für Werkstoffkunde und Werkstoffmechanik, 85748 Garching — [3]TU München, FRM II, 85747 Garching — [4]KIT, Institut für Nanotechnologie (INT), 76344 Eggenstein-Leopoldshafen

Nickel-based superalloys have a huge field of applications, particularly in the high-temperature regions of gas turbines. For those applications the reliable knowledge of residual stresses on different length scales is crucial since they affect the material properties strongly. Beside macroscopic stresses, which influence directly the life time of components, intergranular strains should be taken into account as well, since they always superpose the macroscopic stress state. Those type II stresses, which reflect the micromechanical material behavior, are strongly dependent on the microstructure of the samples.

In this contribution, we present results of mechanical in-situ neutron diffraction tests on the two nickel-based superalloys Inconel 718 and Haynes282. Our data show, that the micromechanical behavior and thus the mechanisms of plastic deformation differ for IN718 and Haynes282. The neutron diffraction results will be discussed in detail with respect to the different observed microstructures, which were characterized in detail by means of electron microscopy like SEM and TEM.

MM 6.3 Mon 10:45 IFW D

Microstructural investigation on the Na2SO4 - NH4Cl salt spray tested Alloy 602CA sheets subjected to different surface modification techniques — •Sai Rajeshwari K[1], Gerhard Wilde[2], Vijay K. Vasudevan[3], and Sankaran S[1] — [1]Department of Metallurgical and Materials Engineering, IIT Madras, Chennai, India — [2]Institute of Materials Physics, University of Münster, Germany — [3]Department of Chemical and Materials Science Engineering, University of Cincinnati, USA

Alloy 602CA is a high temperature corrosion resistant nickel base super alloy with high creep strength in carburizing and oxidizing atmosphere. Alloy 602CA contains 5% (by volume) of Cr23C6 precipitates which act as reservoirs for the formation of a protective Cr2O3 coating in the event of high temperature exposure to oxidation or corrosion. Hence, it is extensively used in thermal, petrochemical and power plant equipment. Corrosion due to Na2SO4 salt deposition is a major challenge and involves high cost.An attempt is made to improve the high temperature corrosion resistance and fatigue properties of the Alloy 602CA sheets through two surface modification techniques namely, High Reduction Cold Rolling (HRCR) and Ultrasonic Nanocrystal Surface Modification (UNSM).Microstructural and corrosion behavior investigations employing Scanning Electron Microscopy and Energy Dispersive Spectroscopy of HRCR and UNSM treated alloy 602CA sheet samples subjected to Na2SO4 :NH4Cl (80:20)salt spray tests for varying duration of 20, 40 and 60 hours at 925°C will be discussed in detail.

MM 6.4 Mon 11:00 IFW D

Tungsten fiber reinforced tungsten (Wf / W) produced by CVD and CVI — •Leonard Raumann[1], Jan Willem Coenen[1], Johan Riesch[2], Hanns Gietl[2], and Christian Linsmeier[1] — [1]Institut für Energie und Klimaforschung Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Max-Planck-Institut für Plasmaphysik, 85748 Garching b. München

Due to excellent thermal and hydrogen retention properties, tungsten is the main candidate for first wall and divertor materials in future fusion reactors. However, the intrinsic brittleness of tungsten is a concern regarding high transient heat loads and neutron irradiation in the fusion environment. To overcome this drawback, tungsten fiber reinforced tungsten (Wf/W) composites are being developed relying on an extrinsic toughing principle. One processing route is the chemical vapor deposition and infiltration of tungsten fiber fabrics. The major challenge for this route is to prevent voids within the composite, which can easily occur if the tungsten film growth separates not yet infiltrated domains from gas flow supply. To achieve fully dense materials the underlying principles have to be fully understood. To asses this process parameters are varied in simplified experimental setups to bring a simulation model in line with the experimental data. The model is taking into account the kinetics for adsorption of the reactants, surface reactions, film growth and desorption of the side products. All are influenced by temperature, pressure, gas mixing ratio and gas flow velocity as well as the substrate geometry and related transport mechanisms. First experimental and theoretical results will be presented.

MM 7: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I

Time: Monday 10:30–13:00 Location: GER 38

MM 7.1 Mon 10:30 GER 38

DFT wants U: Embedded-cluster calculations of surface oxygen vacancies at TiO_2 with Hubbard-corrected DFT — •Matthias Kick, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Surface oxygen vacancies, in particular their nature as charge trapping centers, play an inportant role for many oxide materials properties. However, addressing them with first-principles density-functional theory (DFT) computations remains a challenge. At least Hubbard corrected DFT+U is required to achieve an appropriate electron localization. At the same time, the large dielectric constant of polarizable oxides like TiO_2 leads to a strong polarization response. As a result supercells of increasing size are necessary in order to avoid spurious interactions between periodic images in case of charged defects, rendering the conventional periodic boundary condition supercell approach impractical.

Full DFT+U functionality has been implemented in the all-electron electronic structure code FHI-aims. Combined with the solid state (QM/MM) embedding functionality in FHI-aims, this yields a numerically most efficient approach to treat aperiodic aspects at oxide surfaces. We illustrate this by calculating neutral and charged states of the surface oxygen vacancy at rutile TiO_2 (110). We systematically assess the reliability and computational efficiency by comparing to hybrid-level DFT calculations and calculations performed in conventional supercells.

MM 7.2 Mon 10:45 GER 38

Hubbard interactions from density-functional perturbation theory — •Iurii Timrov, Matteo Cococcioni, and Nicola Marzari — Theory and Simulation of Materials (THEOS), and NCCR-MARVEL, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

DFT+U, together with its V and J extensions, is a simple and powerful tool to model systems containing partially-filled manifolds of localized states [1]. However, the Hubbard parameters are often - and in our view incorrectly - treated semi-empirically. Conceptual and practical methods to determine e.g. the Hubbard U parameter have nevertheless been introduced long ago, based either on the constrained random-phase approximation (cRPA) or on linear-response theory [2]. These approaches make DFT+U a fully first-principles and self-contained method, but are often overlooked due to their cost or complexity. Here, we introduce a computationally inexpensive and straightforward approach to determine the linear-response U, hitherto obtained from the difference between bare and self-consistent inverse electronic susceptibilities evaluated from supercell calculations. By recasting these calculations in the language of density-functional perturbation theory we remove the need of supercells, and allow for a fully automated determination of susceptibilities and Hubbard parameters. Such developments open the way for deployment in high-throughput studies, while providing the community with a simple tool to calculate consistent values of U for any system at hand. [1] V. Anisimov et al., PRB 44, 943 (1991), [2] M. Cococcioni et al., PRB 71, 035105 (2005).

MM 7.3 Mon 11:00 GER 38

Time-evolution using full configuration interaction quantum Monte Carlo — •Kai Guther[1], Werner Dobrautz[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We report on a new method to perform real-time quantum evolution of a fermionic system using the full configuration interaction quantum Monte Carlo method [1]. To stabilize the algorithm, a slow simultaneous imaginary-time evolution is performed, yielding properties for times slightly rotated into the complex plane.

We employ this technique to compute Green's functions and therefore by means of analytic continuation also spectral weight functions. We demonstrate the applicability of the algorithm using the examples of the 2D-Hubbard model and the carbon dimer, showing that the algorithm can in principle be used as an Anderson solver for DMFT and is capable of obtaining photoemission spectra of ab-initio systems.
[1] G.H. Booth, A.J.W. Thom and A. Alavi, J. Chem. Phys. 131, 054106 (2009)

MM 7.4 Mon 11:15 GER 38

Laplace-transformed MP2 with localized Resolution of Identity for molecular and periodic systems — •Arvid Ihrig, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut, Berlin, Germany

The self-interaction error is a well-known problem in (semi)local functionals in density-functional theory (DFT) and to a lesser extend also in hybrid functionals. It leads to a quantitatively and sometimes even qualitatively wrong description. One possible remedy is the 2nd order Moller-Plesset perturbation theory (MP2) and the double-hybrid DFT methods based on it. However, the time and memory requirements prevent their routine-usage for large molecular and condensed-matter systems.

In this work we combine our localized Resolution of Identity (RI-LVL) [1] and its favourable memory requirements with the low-order scaling of the Laplace-transformed MP2 (LT-MP2) [2]. Our highly parallelizable LT-MP2 implementation in a numeric atom-centered orbital (NAO) framework allows us to treat both cluster and periodic models in the same computational environment. We demonstrate the accuracy and other features of our implementation for examples of water clusters and TiO_2 surfaces with small absorbed molecules. We furthermore present a way how the distance-dependent integral screening [3] from the Ochsenfeld group can be generalized to periodic systems.

[1] Ihrig et al., New J. Phys. 17, 093020 (2015)
[2] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[3] S. Maurer et al., J. Chem. Phys. 136, 144107 (2012)

MM 7.5 Mon 11:30 GER 38

Bond Disproportionation in Rare-Earth Nickelates: Describing Lattice Distortions within DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, RNiO$_3$, display a rich and only partially understood phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT), that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and can (in the simplest picture) be understood as a charge disproportionation of the Ni^{3+} cations into Ni^{2+} and Ni^{4+}. Here, we use density functional theory (DFT) and its extensions (DFT+U, DFT+DMFT) combined with symmetry-based distortion mode analysis to explore the interplay between lattice distortions, magnetic order and electronic correlation effects in rare-earth nickelates. Thereby, we want to explore the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom by comparing with DFT+U results and available experimental data.

MM 7.6 Mon 11:45 GER 38

Density matrix embedding theory for coupled fermion-boson systems — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], Joshua S. Kretchmer[2], Garnet K. L. Chan[2], and Angel Rubio[1,3] — [1]Max Planck Institut für Struktur und Dynamik der Materie, Hamburg — [2]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian

We analyze strongly correlated fermion-boson systems by extending Density Matrix Embedding Theory (DMET) from the purely electronic case [1] to coupled fermion-boson systems. DMET is a novel embedding theory which uses the Schmidt decomposition to divide the treated system into an impurity and a bath part. We project the bath part into the part of the Fock space that contains the entanglement with the impurity region and then solve this much smaller entangled system with exact diagonalization and DMRG.

With this technique, we treat lattice systems of Hubbard-Holstein type, where fermions and bosons are coupled by a bilinear Froehlich coupling. As we choose coherent states for the bosonic basis set, it is convenient to apply our approach to electron-phonon as well as to electron-photon systems.

By using a DMRG solver for the DMET algorithm, an accurate treatment of 2 dimensional systems becomes feasible.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

MM 7.7 Mon 12:00 GER 38

Vertex function of homogeneous electron gas — •Yaroslav Pavlyukh — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

We present a systematic study of the vertex function correction in homogeneous electron gas at metallic densities [1]. Contrary to a popular belief the vertex function not only provides corrections to the well known plasmon or particle-hole pair scatterings, but also gives rise to new physical processes such as generation of two plasmon excitations or the transformation of the initial one-particle state into a two-particles-one-hole state. Using a merger of the many-body perturbation and scattering theories, which is a distinct feature of our method, it is shown that additional scattering channels are responsible for the bandwidth reduction (as observed in photoemission experiments on bulk sodium), appearance of the secondary plasmonic satellite below the Fermi level and lead to a substantial modification of the electron spectral function.

[1] Y. Pavlyukh, A.-M. Uimonen, G. Stefanucci, R. van Leeuwen, Phys. Rev. Lett. **117**, 206402 (2016)

MM 7.8 Mon 12:15 GER 38

Coupled-Cluster approaches for molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

As a well-established and successful wave-function theory hierarchy in quantum chemistry, the coupled-cluster (CC) ansatz is attracting increasing attention in computational materials science [1]. However, compared to traditional density-functional approximations, CC approaches face much greater challenges regarding numerical implementation, bassis-set accuracy and efficiency, in particular for solids [2]. In this report, we present a highly parallel implementation of the CC approaches with singles, doubles and perturbative triples, CCSD(T), in the numeric atom-center orbital (NAO) framework. This implementation allows CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. Taking some popular quantum-chemistry test sets (S22, ISO34, and CYCONF), we demonstrate that CCSD(T) with correlation-consistent NAO basis sets [3] can provide accurate reference data for molecular properties. Our solid-state examples include elemental and binary crystals, as Ne (fcc), C, Si (diamond), LiF, MgO (rocksalt), and BN (zincblende).

MM 7.9 Mon 12:30 GER 38

Implementation of the SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach — •Werner Dobrautz[1] and Ali Alavi[1,2] — [1]Max-Planck-Institut für Festkörperforschung — [2]Department of Chemistry, University of Cambridge

The Full Configuration Interaction Quantum Monte Carlo (FCIQMC) algorithm [1] is a projector QMC method, previously formulated in the total anti-symmetric space of Slater Determinants, based on the imaginary-time Schrödinger equation to obtain the ground state of a system in the long-time limit.

By formulating the method in eigenfunctions of the $\hat{S}^2$ spin-operator via the Graphical Unitary Group Approach [2] we can make use of the block-diagonal form of spin-preserving, non-relativistic Hamiltonians for different values of the total spin. This allows us to lift possible near degeneracies of low-lying excitations of different spin sectors, calculate spin-gaps more easily and obtain the physical correct ground-state, without spin-contamination, and identify its total spin quantum number.

Our method does not rely on expanding the spin-eigenfunctions in linear combinations of Slater Determinants and thus does not hit an exponential bottle neck and can be applied to system sizes larger than previously reachable with similar approaches.

[1] G. Booth, A. Thom and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)
[2] I. Shavitt, Int. J. Quantum Chem. Symp., **11:** 131 (1977); Int. J. Quantum Chem. Symp., **12:** 5 (1978)

MM 7.10 Mon 12:45 GER 38

A study of the dense uniform electron gas with high orders of coupled cluster — •Verena Andrea Neufeld and Alex James William Thom — University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We used the recently developed stochastic coupled cluster method [Phys. Rev. Lett. (2010) 105, 263004 and J. Chem. Phys. (2016) 144, 084108] to benchmark the dense uniform electron gas (UEG). The aim was to make predictions about what truncation level of coupled cluster is needed to reach sufficient accuracy in electronic correlation energies for a range of electron densities. This will aid our future studies of solids with stochastic coupled cluster.

We take advantage of sparsity in wavefunctions by doing coupled cluster stochastically. In this study, we used coupled cluster truncation levels up to CCSDTQ5, that includes single, double, triple, quadruple and quintuple excitations directly. We considered the 14 electron UEG with Wigner-Seitz radius in the range 0.5 to 5.0 a.u.. We applied coupled cluster truncations from CCSD to CCSDTQ5 and extrapolated to the complete basis set size limit. By comparing the differences in energy calculated with CCSD to CCSDTQ5, we learn what truncation level is necessary for sufficient accuracy. What truncation level is needed, is dependent on the level of correlation, which decreases with electron density. We are therefore able to relate the degree of correlation linked to electron density to the level of coupled cluster needed for accuracy. This information will prove valuable when tackling periodic solids that can be approximated by the UEG.

MM 8: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Segregation and Embrittlement II

Time: Monday 11:45–13:15 Location: BAR 205

MM 8.1 Mon 11:45 BAR 205

Atomistic study of Hydrogen embrittlement of grain boundaries in Nickel — •Ali Tehranchi and William A. Curtin — Laboratory for Multiscale Mechanics Modeling, EPFL, CH-1015 Lausanne, Switzerland

The Hydrogen ingress into a metal is a persistent source of embrittlement. Fracture surfaces are often intergranular, suggesting favorable cleave crack growth along grain boundaries (GBs) as one driver for embrittlement. Here, atomistic simulations are used to investigate the effects of segregated hydrogen on the behavior of cracks along various symmetric tilt grain boundaries in fcc Nickel. The results of the simulations are compared with the theoretical predictions of Rice and Griffith theories. Both simulations and theoretical calculations showed that the presence of segregated hydrogen atoms cannot transform the ductile behavior of an intrinsically ductile crack to brittle behavior. For the intrinsically brittle cracks, hydrogen atoms decrease the critical cleavage load. Thus cleavage-like failure observed in the experiments are presumably caused by mechanisms involving H diffusion or dynamic crack growth.

MM 8.2 Mon 12:00 BAR 205

Defect generation in Palladium by Hydrogen loaded Niobium layers — •Vladimir Burlaka, Vladimir Roddatis, Marian Bongers, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Germany

In this paper, we use layers with high hydrogen affinity to influence the defect structure of an overlaying catalytic layer. It will be shown that pre-existing defects can be healed out by a low-pressure hydrogen treatment and, opposite, additional defects can be generated by a higher pressure treatment. In our study Pd/Nb/Al2O3 double layers are studied during hydrogen gas exposure at room temperature by using Scanning Tunneling Microscopy (STM), X-ray diffraction (XRD) and environmental transmission electron microscopy (ETEM). [1] STM results show hydrogen-induced topography changes at the Pd/Nb interface. The XRD measurements demonstrate that the topography changes in the Nb-H film result in microstructural changes in the overlaying Pd layer. ETEM measurements on cross-cut lamellas show that the modification of the Pd top-layer occurs due to the precipitation and growth of the hydride phase within the Nb underlying film: generation of new defects and interface roughening are observed. We conclude that these changes in the Pd layer can be varied by changing the Nb-film thickness. [2]

Financial support by the DFG via PU131/9 and PU131/12 and the beamtime provided by DESY and ESRF are acknowledged. [1] V.Burlaka, S.Wagner, M.Hamm, A.Pundt, Nano Letters 16 (2016) 6207. [2] V.Burlaka, V.Roddatis, M.Bongers, A.Pundt, submitted.

MM 8.3 Mon 12:15 BAR 205

Confined topological impurity segregation at faceted Si grain boundaries — •Christian Liebscher[1], Andreas Stoffers[1], Oana Cojocaru-Mirédin[2], Baptiste Gault[1], Christina Scheu[1], Gerhard Dehm[1], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]RWTH Aachen, Institute of Physics (IA), 52056 Aachen, Germany

Coincident site lattice (CSL) boundaries and trace impurities of Carbon (C) and Iron (Fe) are degrading the electrical performance of multicrystalline Silicon (mc-Si) by promoting charge carrier recombination. Our study provides unprecedented insights into the connection of the faceted nature of grain boundaries in mc-Si and confined impurity segregation. The direct correlation of atomic resolution aberration-corrected scanning transmission electron microscopy (STEM) and 3D atom probe tomography (APT), obtained by probing exactly the same specimen position in both instruments establishes segregation of Carbon (C) and Iron (Fe+N) to linear junctions of merging grain boundary facets. Both, the segregation patterns of C and (Fe+N), as observed by APT, form linear segregation tubes that decorate facet junctions of a $\Sigma3$ grain boundary with a facet length between 2 and 10 nm. By observing the atomic structure of a $\Sigma9$ grain boundary with a facet length of 10 to 50 nm on an APT needle by STEM followed by subsequent 3D chemical analysis directly verifies the confined impurity segregation that is driven by the grain boundary topology.

MM 8.4 Mon 12:30 BAR 205

stInvestigations on Grain boundary Segregation in Nanocryalline Materials with Atom Probe Tomography — •Rüya Duran and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

Nanomaterials are not just opening new opportunities for improvement of materials, but also challenges in characterizing and understanding the changed atomic structures and the chemical and physical behavior within the material. Grain boundaries have the major influence on the properties. An important property is the segregation at these defects. The grain boundary interacts with solute atoms which change their chemical composition and change the boundary and so, the material properties. In this work, the temperature and concentration dependence of grain boundary segregation in Cu/Ni thin films is investigated. For the analysis the Atom Probe Tomography (APT) is used. With the APT a very high spatial resolution in all three dimensions is achieved which makes the analysis of such a fine defect more precise. Since the APT allows chemical analysis in single atom sensitivity, segregation to grain boundaries can be easily identified. With the knowledge of the chemical composition, concentration profiles can be formed from which the widths and also the amplitudes of the segregation zones can be determined. With a new evaluation method the data will be extracted by using a model function for the defect which is fitted to the point data to increase the spatial resolution and to avoid artefacts.

MM 8.5 Mon 12:45 BAR 205

Macroscopic and microscopic investigation of Sulphur - induced embrittlement in Copper — •Thorsten Meiners, Zirong Peng, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Sulphur (S) is a common impurity element, which has a very low solubility in copper alloys (Cu) and is attributed to cause grain boundary (GB) embrittlement by segregating to the boundaries. In our study, macro-tensile tests at room temperature (RT), 200 °C and 400 °C are applied to investigate embrittlement of polycrystalline Cu alloys containing 14, 27 and 7900 ppm of S, named alloy 1, 2 and 3 here. Alloy 1 shows a reduction in ductility of 18% from RT to 400 °C. Compared to that, alloy 2 shows a reduction in ductility of 29% at RT and 70% at 400 °C and alloy 3 58% at RT and 67% at 400 °C. The grain size was determined to about 2 mm using electron backscatter diffraction. Alloy 1 is free of precipitates and high resolution transmission electron microscopy (TEM) and atom probe tomography reveal no segregation of S to random GBs. In alloy 2, small precipitates on the order of 50nm can be established at the GBs and within the grains with scanning electron microscopy. Alloy 3 shows a dendritic structure where large low chalcocite Cu2S precipitates (several micro meters) are located at the dendrites and small precipitates (about 50 nm) are located in interdendritic regions. For the alloys 2 and 3 high-resolution TEM does also not confirm segregation of S to the random GBs and the embrittlement of the alloys is mainly related to the presence of precipitates.

MM 8.6 Mon 13:00 BAR 205

Silver segregation induced nanofaceting of an asymmetric tilt

grain boundary in copper — •Nicolas J. Peter, Christian H. Liebscher, Raheleh Hadian, Blazej Grabowski, Christoph Kirchlechner, and Gerhard Dehm — Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Grain boundary faceting is a thermally activated process. It can be suppressed on experimental time scales depending on temperature and driving force. We show here that chemistry can be used to intentionally trigger faceting.

The present study investigates the segregation of Ag to an asymmetric tilt boundary in Cu. Aberration-corrected high-resolution scanning transmission electron microscopy reveals that annealing the Ag coated bicrystal at 800°C for 120 h results in the formation of nanometer-sized, regularly spaced, symmetric Sigma 5 (210) segments within the overall asymmetric boundary. We confirm that reference samples without Ag, annealed under the same conditions, show no thermally activated faceting, even down to the atomic level.

Our observations oppose an anticipated trend to form coarse facets or change the overall boundary plane orientation to lower energy Sigma 5 (210) or (310) planes. Atomistic simulations on specifically chosen reference boundaries support the experimental observations and reveal the atomistic mechanisms of the chemically induced nanofaceting.

Migration paths and atomic column occupancies are extracted over time to allow for a first quantification approach of such a system, thereby showing the stability of the induced Ag containing nanofacets.

MM 9: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses II - Undercooled Melts

Time: Monday 11:45–13:15 Location: IFW A

MM 9.1 Mon 11:45 IFW A

Short range order in liquid metals — Guy Makov[1] and •Eyal Yahel[2] — [1]Materials Dept, Ben-Gurion University of the Negev, Beer Sheva, Israel — [2]Physics Dept, NRCN, Beer Sheva, Israel

Evolution of short range structure in liquid metals as a function of temperature in the regime from supercooled to high temperature melt is studied within the quasi-crystalline model of liquid structure. Experimental data on elements of groups IV and V, many of which exhibit anomalous thermophysical properties are compared with molecular dynamics generated data on model systems.

The quasi-crystalline model allows quantitative characterization of the short range order in liquids by identifying a reference structure. It is found that the liquid pnictides are characterized by a short range order which reflects a Peierls distorted structure. This distortion decreases as the elements progress down the periodic table column V and explains the large change in coordination number from 3 to 8. Surprisingly the distortion is found to increase with temperature and correlates with the appearance of a sound velocity maximum with respect to temperature. Column IV elements exhibit a very different short range order which is found to remain constant with temperature, possibly indicating that the origin of the sound velocity anomaly in these systems is not related to any structural rearrangement of the liquid unlike in the pnictides. Simple models allow supercooling into the glassy state with modification of the short range order into intermediate states between the liquid and solid phases.

MM 9.2 Mon 12:00 IFW A

Influence of the Chemical Short-Range Order on the Atomic Dynamics in Binary Glass-Forming Melts — •Benedikt Nowak[1], Dirk Holland-Moritz[1], Fan Yang[1], Thomas Voigtmann[1], Tobias Kordel[1], Thomas Hansen[2], and Andreas Meyer[1] — [1]Institute of Materials Physics in Space, German Aerospace Center (DLR), 51170 Cologne, Germany — [2]Institut Laue-Langevin (ILL), 38042 Grenoble, France

The dynamical behaviour of atoms and their short-range order are crucial for understanding the glass-forming ability of metallic melts. To investigate the short-range order (SRO) we measured partial structure factors for the melts of Zr-Ni by combining electrostatic levitation with neutron diffraction and isotopic substitution [1]. Mode coupling theory (MCT) allows us to establish structure-dynamics relations using partial structure factors as an input [2]. The self-diffusion coefficients derived by MCT show the same trends with respect to composition and temperature dependence compared to experimental results.

MCT results highlight that diffusion is partly coupled, exhibiting a distinct composition dependence of the ratio of diffusion coefficients. Compared to a hard-sphere model, we show that such a composition dependent decoupling is due to the strong chemical interaction between Zr and Ni atoms. This can be understood by the fraction of different atomic nearest-neighbour pairs, derived from the measured partial structure factors.

[1] D. Holland-Moritz et al., PRB 79, 064204 (2009) [2] Th. Voigtmann et al., EPL 82, 66001 (2008)

MM 9.3 Mon 12:15 IFW A

Self-diffusion in liquid gold-silicon investigated using quasielastic neutron scattering — •Zach Evenson[1], Fan Yang[2], Giovanna Simeoni[1], and Andreas Meyer[2] — [1]Maier-Leibnitz Zentrum (MLZ) and Physik Department, Technische Universität München — [2]Institute for Materials Physics in Space, German Aerospace Center, Cologne

We use incoherent quasi-elastic neutron scattering to study the atomic dynamics of gold in a eutectic Au81Si19 melt. Despite the glass-forming nature of this system, the gold self-diffusivity displays an Arrhenius behavior with a low activation energy characteristic of simple liquids. At high temperatures, long-range transport of gold atoms is well described by hydrodynamic theory with a simple exponential decay of the self-correlation function. On cooling towards the melting temperature, structural relaxation crosses over to a highly stretched exponential behavior. This suggests the onset of a heterogeneous dynamics, even in the equilibrium melt, and is indicative of a very fragile liquid.

MM 9.4 Mon 12:30 IFW A

Ni-diffusion in a liquid and undercooled NiSi alloy — •Franz Demmel — ISIS Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK

Understanding the dynamics of liquid metals and alloys can be relevant for technological applications like solidification and welding. Here the Nickel self-diffusion coefficient was measured in a Ni75Si25 alloy in the liquid and undercooled state covering a temperature range of 1400K to 1900K. Quasielastic neutron scattering on a 2.7 mm diameter spherical sample was used to deduce the Ni self-diffusion coefficient. The experiment was performed by applying aerodynamic levitation with CO2 laser heating. That containerless technique allowed an undercooling of about 100K over 4 hours of measurement time. The temperature dependence of the diffusion coefficients follows an Arrhenius type behavior. The derived activation energy for the diffusion process is about 10% larger than in pure Nickel and is probably the reason for the moderately slower self-diffusion coefficients compared to pure Ni. Surprisingly, molecular dynamics simulations predicted a change in dynamics from an Arrhenius-type behavior to a power-law for temperatures as high as twice the glass transition temperature [1]. Our data are compatible with a power-law behavior for the Ni self-diffusion [2]. [1] Y.J. Lu, H. Cheng and M. Chen, J. Chem Phys 136 214505 (2012) [2] F. Demmel, L. Hennet, S. Brassamin, D.R. Neuville, J. Kozaily and M. Koza, Phys Rev B 94 (2016) 014206

MM 9.5 Mon 12:45 IFW A

Dynamic viscosity of Ge-Sb-Te alloys in liquid and supercooled liquid state — Hans Weber[1,2], Mathias Schumacher[3], Pal Jovari[4], Werner Skrotzki[2], Riccardo Mazzarello[3], and •Ivan Kaban[1] — [1]IFW Dresden, Institute for Complex Materials, Germany — [2]TU Dresden, Institute of Structural Physics, Germany — [3]RWTH Aachen University, Institute for Theoretical Solid State Physic, Germany — [4]Institute for Solid State Physics and Optics, Budapest, Hungary

Dynamic viscosity of binary Ge-Te and ternary Ge-Sb-Te alloys is measured by the oscillating-cup method and calculated by ab-initio molecular dynamics (AIMD) simulations. Binary alloys around Ge15Te85 eutectic composition show a strong deviation from Arrhenius plot at about 100-150 K above the melting temperature. In contrast, viscosity of GeTe and Ge-Sb-Te alloys shows Arrhenius behavior in the liquid and weakly supercooled liquid state, whereas it seems to be strongly non-Arrhenius at larger supercoolings. Atomic dynamics and glass-forming ability will be discussed in relationship to the structure of the alloys studied.

MM 9.6 Mon 13:00 IFW A

Self-diffusion in liquid Al-Ge investigated with quasi-elastic neutron scattering — •Sandro Szabo[1,2] and Zachary Evenson[1,2] — [1]Research Neutron Source FRM II, Garching, Germany — [2]Technische Universität München, Munich, Germany

Self-diffusion of atoms in liquid metals can be investigated on an absolute scale with quasi-elastic neutron scattering (QENS). For the Al-Ge system accurate modeling of solidification processes and mass transport in general suffers due to the lack of experimentally determined temperature-dependent diffusion coefficients. We investigate the self-diffusion of Ge in liquid Al-Ge in a wide temperature range at and below the melting point of the respective pure elements. QENS measurements were carried out at the multi-disc chopper time-of-flight spectrometer TOFTOF at the research neutron source Heinz Maier-Leibnitz (FRM II). The QENS results show a standard deviation of the self-diffusion coefficients of only 4 %, which is significantly more precise when compared to classical measurements in long capillaries. In all investigated Al-Ge alloys, the self-diffusivity of Ge follows an Arrhenius behavior over the entire investigated temperature range. At the melting point of pure Ge, the self-diffusivity of Ge in the investigated alloys is higher by some 22-28 % than that of pure Ge. This is in line with existing findings concerning dendrite growth in this system during solidification. Accurate calculations of mass flow, which were previously impeded by the lack of accurate diffusion data, might now be possible.

MM 10: Computational Materials Modelling - Accelerated Approaches

Time: Monday 11:45–13:15 Location: IFW B

MM 10.1 Mon 11:45 IFW B

An on-the-fly parameterized redundant internal coordinate preconditioner for quasi-Newton geometry optimization in atomistic calculations — •Christoph Freysoldt and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

We propose a variant of quasi-Newton geometry optimization for atomistic calculations, using an approximate Hessian in terms of internal coordinates (bond lengthes, bond angles) as a preconditioner for a BFGS-type cartesian-coordinate quasi-Newton scheme. The key idea is to parameterize the Hessian on the fly. By automatically classifying all interatomic bonds according to bond length and elements involved, and treating all similar bonds equal, we arrive at a very small number of parameters that can be determined from few displacements, often only one. The superior performance for supercell calculations compared to a standard cartesian-coordinate optimizer is demonstrated.

MM 10.2 Mon 12:00 IFW B

Implementation and testing of a temporal acceleration scheme for kinetic Monte Carlo simulations: The case of CO methanation on stepped metals — •Mie Andersen and Karsten Reuter — Theoretical Chemistry, Technische Universität München, Germany

The efficiency of kinetic Monte Carlo (kMC) simulations is limited by the disparity of the timescales for the processes included in the microkinetic model. A novel algorithm has been developed to overcome this problem by the automatic detection of fast, reversible processes and the scaling of their rate constants with respect to the slower irreversible processes [1]. We have implemented this algorithm in our in-house kMC code 'kmos' [2] and assessed its efficiency and accuracy for the case of CO methanation on stepped metals. By making use of a scaling-relation based approach, we cover the trends over the entire transition metal series, which makes for a range of different test cases for the algorithm. While the algorithm overall performs well, we point out some limiting cases where the algorithm breaks down and discuss strategies for overcoming these issues.

[1] E. Dybeck, C. P. Plaisance, M. Neurock, submitted to J. Chem. Theory Comput. (2016) [2] M. J. Hoffmann, S. Matera, K. Reuter, Comput. Phys. Comm. 185, 2138 (2014)

MM 10.3 Mon 12:15 IFW B

Defect migration in metals by atomistic-continuum coupling — •Liam Huber, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Atomistic simulations provide important insight into the underlying mechanisms which control material behaviour, and are an important part of knowledge-based design for new alloys. However, experimental time- and length-scales often lie beyond the reach of classical molecular dynamics (MD), even with modern advances in computational power. One approach to extend the length-scales accessible is to couple MD to a less expensive continuum model, typically represented using finite elements (FE). We present improvements to the FE-atomic (FEAt) coupling scheme which allow the MD-domain to track the migration of planar, line, and point defects at finite temperatures. By dynamically adapting our MD/FE domain partitioning through refinement and coarsening, we keep defects fully atomistically resolved while maintaining the cost-advantage of the coupled method. We apply this method to study grain boundary migration in Al and the nucleation and motion of dislocations during Al nano-pillar compression.

MM 10.4 Mon 12:30 IFW B

Nested sampling for alloys — •Robert J.N. Baldock[1], Christopher Sutton[2], and Luca M. Ghiringhelli[2] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Theory Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We present a new nested sampling algorithm that enables the calculation of complete composition-temperature phase diagrams of alloys in a single simulation. Multicomponent phase diagrams are obtained in both the semi-grand ensemble, and at fixed overall composition, as a simple post-processing of the same simulation. We demonstrate the method by calculating the fixed pressure phase diagram of an eutectic binary Lennard-Jones system with fully continuous configuration space and an eutectic Ising model. Finally we showcase the approach by calculating the first principles phase diagram of a prototypical transparent conducting oxide (wide bandgap) material, $\left(\mathrm{Zn}_x\mathrm{Mg}_{1-x}\right)\mathrm{O}$, using a lattice model derived from density functional theory.

MM 10.5 Mon 12:45 IFW B

Controlling the energy of defects and interfaces in the amplitude expansion of the phase-field crystal model — •Marco Salvalaglio[1], Rainer Backofen[1], Axel Voigt[1], and Ken Elder[2] — [1]Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, Oakland University, Rochester, 48309 Michigan, USA

The Phase-Field Crystal (PFC) approach describes the dynamics of local atomic probability density on atomic length and diffusive time scales. It generally requires a fine spatial discretization, which limits the application of the method to small systems. The so-called amplitude expansion of the PFC model is known to solve this issue, accounting for the slowly-varying amplitudes of periodic probability densities. However, some restrictions exist in the quantitative description of material properties. In this work, we address the tuning of the interface and defect energy within the amplitude expansion of the PFC model. We extend the standard approach by including an additional energy term accounting for changes in the order of the solid phase. Its effects are investigated by FEM calculations. First, the control of the solid-liquid interface energy is considered as well as the changes induced in the interface morphology. Then, the tuning of the energy of defects is illustrated. The influence of the additional energy term on the dynamics and annihilation of defects is also discussed. We focus here on 2D systems involving crystal lattices with triangular symmetry. The connection of the considered approach to the description of realistic materials is shown for the technology-relevant graphene structure.

MM 10.6 Mon 13:00 IFW B

Ab initio determination of phonon lifetimes at elevated tem-

peratures — •Albert Glensk[1], Blazej Grabowski[1], Tilmann Hickel[1], Jörg Neugebauer[1], Pascal Neibecker[2], Jürgen Neuhaus[2], Michael Leitner[2], Klaudia Hradil[2], and Winfried Petry[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The experimental measurement of phonon dispersions is well established. The corresponding phonon lifetimes (i.e., inverse linewidths) are - in contrast - assessed experimentally only for a handful of materials and are usually restricted to room temperature where anharmonic effects are small. Standard theoretical methods applying perturbation theory have shown to successfully describe the underlying phonon-phonon interactions at low temperatures. However, significant discrepancies to experiment (~100%) are found at elevated temperatures where the phonon broadening due to anharmonicity becomes large [1-2]. Applying the recently developed Local Anharmonic approximation [3] we determine ab initio values for phonon lifetimes in Al for a temperature range up to melting. We discuss its performance in comparison to previous perturbative approaches and our own experimental assessments for this temperature range.

[1] J. Pang et al., PRL 110, 157401 (2013).
[2] X. Tang et al., PRB 84, 054303 (2011).
[3] A.Glensk et al., PRL 114, 195901 (2015).

MM 11: Biomaterials

Time: Monday 11:45–13:30 Location: IFW D

MM 11.1 Mon 11:45 IFW D

Macromolecular HPMA-based drug delivery system - behavior in protein environment — •Xiaohan Zhang[1], Bart-Jan Niebuur[1], Petr Chytil[2], Tomas Etrych[2], Sergey K. Filippov[2], Alexey Kikhney[3], Florian Wieland[3], Dmitri I. Svergun[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie, Garching, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]European Molecular Biology Laboratory, DESY, Hamburg, Germany

Copolymers based on N-(2-hydroxypropyl)methacrylamide (HPMA) having cholesterol side groups self-assemble into ellipsoidal nanoparticles (NPs) in aqueous solutions [1,2]. The core and the shell are formed by cholesterol and by HPMA, respectively. They have been proposed as drug carriers. However, little is known on their behavior in human blood environment.

We use synchrotron small-angle X-ray scattering (SAXS) to investigate HPMA copolymers in an aqueous solution of human serum albumin(HSA), which is very abundant in human blood, to investigate the influence of HSA on the NPs' structure. The length of the NPs is reduced even if very small amounts of HSA are present. We speculate that HSA binds to cholesterol groups and removes them from the NPs.

[1] S. K. Filippov, et al., Biomacromolecules, 2012, 13, 2594
[2] S. K. Filippov, et al., Biomacromolecules, 2013, 14, 4061

MM 11.2 Mon 12:00 IFW D

Dealloying-based nanoporous metallic materials for orthopedic implant applications — •Ilya Okulov[1], Artem Okulov[1,2], Berengere Luthringer[3], Jürgen Markmann[1], Regine Willumeit-Römer[3], and Jörg Weissmüller[1] — [1]HZG, Institute of Materials Research, Division of Materials Mechanics, Germany — [2]Institute of Metal Physics, Ural Branch of RAS, Russia — [3]HZG, Institute of Material Research, Division of Metallic Biomaterials, Germany

The close match of stiffness between orthopedic implant material and bone is critically important to ensure fast healing of injured tissues. Here, we propose a design strategy to develop metallic materials possessing Young's modulus matching that of human bone using liquid metal dealloying (LMD). LMD is a process of selective dissolution of one or several elements from the solid precursor into the liquid metal, while the remaining elements simultaneously organize and form a porous structure. To demonstrate our strategy, we developed interpenetrating-phase Ti-Mg composites and microporous TiZr alloys by LMD. The Young's modulus of the microporous TiZr alloys is adjustable in a range of 3.2 to 15.1 GPa by controlling metal fraction. The Young's modulus of the Ti-Mg composites can be as low as 25 GPa. These low values of Young's modulus become interesting in a view of high yield strength of the microporous TiZr and the Ti-Mg composites reaching up to 480 MPa and 450 MPa, respectively. This strongly suggests opportunities as future advanced implant materials will significantly enhanced performance.

MM 11.3 Mon 12:15 IFW D

In-situ SEM / TEM fracture tests on (modified) pine sap wood — •Mona-Christin Maass[1], Maximilian Wentzel[2], Holger Militz[2], and Cynthia Volkert[1] — [1]Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany — [2]Wood Biology and Wood Products, Georg-August-University of Göttingen, Büsgenweg 4, Göttingen, Germany

There is evidence that intrawall failure of wood occurs at the interface between the S1 and S2 cell wall layer. However, up to now, the fracture mechanisms of the cell wall remain unexplored. Therefore, we performed fracture tests of pine wood tracheid cell walls which are important because pine – mostly made of tracheid cells – is very common. Our experimental setup enables us to create a crack in the cell wall and to observe the crack propagation in-situ with an electron microscope.

We have observed that crack propagation is not continuous, but intermittently starts and stops accompanied with a change in propagation direction. We attribute this intermittent behavior to the abrupt change of the microfibril angle at the interface between the S1 and S2 cell wall layer and propose that the resultant increase in toughness is a driving force for the natural adaptation of the layered structure. Additionally, we will investigate pine sap wood that has been heat-treated or modified with a methylol resin. The treated wood has higher resistance against fungi but reduced bending and tensile strength relative to untreated wood. Here, the goal is to understand the reasons for the poorer mechanical properties on the basis of the crack behavior.

MM 11.4 Mon 12:30 IFW D

Nanoscale mechanical properties of wood: Effects of heat treatment and sample preparation — •Salimeh Saleh[1], Dominik Tönnies[1], Maximilian Wentzel[2], Holger Militz[2], and Cynthia Volkert[1] — [1]Institute of Materials Physics, University of Göttingen, Germany — [2]Department of Wood Biology & Wood Products, University of Göttingen, Germany

The mechanical properties of wood depend on both the complex hierarchical cellular structure and on the mechanical behavior of the constituent materials. Here, we use nanoindentation to investigate the local mechanical properties of the cell walls, with the goal of understanding how they contribute to the bulk mechanical behavior of wood. Quantitative nanoindentation studies require however a smooth specimen surface. Up until now, this has usually been achieved by using specific embedding materials that unfortunately enter the cell wall, thereby changing their mechanical properties. Here, we investigate methods to prepare suitable nanoindentation specimens using (ultra) microtome from Pine wood and Eucalyptus wood that is either unembedded or embedded with materials such as paraffin that do not enter the cell walls. The Eucalyptus wood is an untreated state and heat-treated at various temperatures and water vapor pressures. We observe that the wood samples become highly heterogeneous after heat treatment: In some regions the elastic modulus is high (~100 GPa), while in other regions it is low (~5 GPa). A possible explanation is that the cellulose becomes spatially localized after heat treatment.

MM 11.5 Mon 12:45 IFW D

Electrospinning biopolymer nanofiber mats for medical and biotechnological applications — •Sarah Vanessa Homburg, Timo Grothe, Nils Grimmelsmann, and Andrea Ehrmann — Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, Bielefeld, Germany

Electrospinning enable creating nanofiber mats from diverse polymers by "dragging" fibers from a polymer solution by a high electric field and depositing them on a substrate. Fiber properties can be controlled by spinning and solution parameters.

While several polymers need toxic or other hazardous solvents, biopolymers can often be spun from aqueous solutions. Additionally, several biopolymers can be used in diverse medical and biotechnological applications, e.g. for tissue engineering, enhanced wound healing, or controlled drug release, but also as filters in different industries. On the other hand, water-soluble nanofiber mats necessitate an additional crosslinking step for most applications.

The presentation gives an overview of the electrospinning principle, spinnable biopolymers and the challenges of crosslinking water-soluble fibers. Possibilities of co-spinning different polymers allowing fiber creation from unspinnable polymers are shown. Physical and chemical properties of nanofibers from different polymers and polymer blends are given.

MM 11.6 Mon 13:00 IFW D

Impact of coordination on the mechanical behavior of polymeric structures — •Huzaifa Shabbir[1] and Markus Hartmann[2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

(Reversible) cross-linking is a common strategy to specifically tailor the mechanical properties of polymeric systems. Often, these cross-links are weaker than the covalent bonds holding the structure together. The reversibility of cross-links provides self healing.

In the current study, Monte Carlo simulations are used to study the influence of the coordination of cross-links on the mechanical properties of polymeric systems. In the simulations, the number of monomers participating in one cross-link defines its coordination. Recent theoretical and simulation approaches deal mostly with two fold coordinated cross-links only [1,2]. Here we aim at closing this gap by explicitly manipulating the coordination of cross-links using an effective description with REBO like interactions.

The results show that the presence of cross-links dramatically increase the stiffness and toughness of the investigated structures. Compared to two-fold coordinated structures, three-fold coordinated cross-links show smoother load-displacement curves and show in general a much richer mechanical behavior due to the increased number of possible bond topologies.

[1] Nabavi et al., Soft Matter 12, 2047 (2016) [2] Nabavi et al., Phys. Rev. E 91, 032603 (2015)

MM 11.7 Mon 13:15 IFW D

Surface, interface and bulk sensitive x-ray absorption spectroscopy probed by total electron yield in liquid cell — •Daniela Schön[1,2], Jie Xiao[1], Ronny Golnak[1], Marc F. Tesch[1], and Emad F. Aziz[1,2] — [1]Institute of Methods for Material Development, Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [2]Freie Univeristät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

Total electron yield (TEY) is often adopted as a probing method for x-ray absorption spectroscopy (XAS). One electrode connecting to sample surface and measuring sample drain current is a common practice to obtain TEY-XA spectra, which makes the TEY method surface sensitive, owing to the short mean-free-path of photoelectrons. In this study, we demonstrate that the interface and bulk sensitive XAS can be individually probed by TEY as well when two electrodes are connected to the front and back sides of a liquid cell. The interfacial dipole layer is argued to be the key factor that separates the x-ray excited electron-hole pairs at interface and generates the resulting electric current which is eventually detected by ammeter as the TEY signal. The mobility and long-distance transportability of positive ions in liquid provides an indispensable assistance to realize the current flow in the liquid bulk. In the two-electrode connection scheme, the acquired current signal produces intensity peaks and dips for the interface and bulk species, respectively, upon the resonant excitations at their corresponding absorption edges.

MM 12: Invited talk Todorova

Time: Monday 15:00–15:30 Location: BAR 205

Invited Talk MM 12.1 Mon 15:00 BAR 205

From weakened chemical bonds to materials breakdown: An ab initio perspective — •Mira Todorova — Max-Planck-Insitut für Eisenforschung, Düsseldorf, Germany

Materials failure mechanisms originate at the microscopic scale. Density functional theory (DFT) calculations have proven to be a versatile tool, providing access to the most fundamental level of forming, weakening or breaking of chemical bonds. A major challenge in the practical realization is the structural and chemical complexity of real-world materials. As will be discussed, fully ab initio computed chemical potentials open a powerful way of transferring the inherently microscopic DFT results to the engineering/device scale. It will be shown that these potentials can be utilised to successfully address various phenomena related to materials failure. The presentation will exemplify this by outlining the steps and the insight which can be achieved by applying these approach on two key failure mechanisms - liquid metal embrittlement [1] and corrosion of galvanized steels [2].

[1] K.-D. Bauer, M.Todorova, K. Hingerl, and J. Neugebauer, Acta Mater. **90**, 69 (2015).

[2] M.Todorova and J. Neugebauer, Farad. Discussions **180**, 97 (2015).

MM 13: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II

Time: Monday 15:00–18:15 Location: GER 38

Invited Talk MM 13.1 Mon 15:00 GER 38

Towards efficient orbital-dependent density functionals for weak and strong correlation — •Igor Ying Zhang[1], Patrick Rinke[1,2], John P. Perdew[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Aalto University, Finland — [3]Temple University, USA

We present a new paradigm for the design of exchange-correlation functionals in density-functional theory [1]. Electron pairs are correlated explicitly by means of the recently developed second order Bethe-Goldstone equation (BGE2) approach [2]. Here we propose a screened BGE2 (sBGE2) variant that efficiently regulates the coupling of a given electron pair. sBGE2 correctly dissociates H_2 and H_2^+, a problem that has been regarded as a great challenge in density-functional theory for a long time [3]. The sBGE2 functional is then taken as a building block for an orbital-dependent functional, termed ZRPS, which is a natural extension of the PBE0 hybrid functional. While worsening the good performance of sBGE2 in H_2 and H_2^+, ZRPS yields a remarkable and consistent improvement over other density functionals across various chemical environments from weak to strong correlation. [1] IY Zhang et al., Phys. Rev. Lett. 117, 133002 (2016); [2] IY Zhang et al., New J. Phys. 18 073026 (2016); [3] AJ Cohen et al., Chem. Rev. 112 289 (2011).

MM 13.2 Mon 15:30 GER 38

Towards a functional for strong correlation via semiclassical model for the indirect energy and local interpolation along the adiabatic connection — •Stefan Vuckovic and Paola Gori-Giorgi — Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands

Finding an approximate XC functional that is able to capture strong correlation effects is a big, unsolved DFT challenge. Even a bigger challenge is to find a functional able to treat any correlation regime successfully. We attempt to construct an XC functional that has no bias towards a particular correlation regime by using a local interpolation along the adiabatic connection between the weak and the strong coupling limit of DFT. [1] In addition to this approach, I will also present our semiclassical model for accurate indirect energies. I will discuss how this model can be used for a construction of XC functionals, exploiting its XC energy density in the conventional gauge, the one of the electrostatic potential of the XC hole.

1. Stefan Vuckovic, Tom J. P. Irons, Andreas Savin, Andrew M. Teale, and Paola Gori-Giorgi, Journal of Chemical Theory and Computation 2016, 12 (6), 2598-2610

MM 13.3 Mon 15:45 GER 38

Benchmark of GW approaches for the GW100 test set — •Patrick Rinke[1], Matthias Dauth[2], Fabio Caruso[3], and Michiel van Setten[4] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]University of Bayreuth, Germany — [3]University of Oxford, England — [4]Université Catholique de Louvain, Belgium

Many-body theory in the GW approach has become the method of choice for calculating charged excitations in solids. Now it is increasingly being applied to molecules, but fundamental questions regarding its *modus operandi* and its accuracy remain. To address both of these aspects, we present a comprehensive assessment of different GW methodologies for the recent GW100 test set [1] of molecular ionization energies [2]. We compare our GW calculations to coupled-cluster singles, doubles, and perturbative triples [CCSD(T)] reference data for GW100. We find ionization energies of fully self-consistent GW and quasiparticle self-consistent GW in excellent agreement with CCSD(T), with discrepancies typically smaller than 0.3 eV and 0.2 eV, respectively. For partially self-consistent and perturbative GW the deviation from CCSD(T) is strongly dependent on the starting point. An optimal starting point is found by minimizing the deviation from the straight-line error [3], which concomitantly yields a systematic improvement of the ionization energies. [1] M. J. van Setten, P. Rinke, *et al.*, J. Chem. Theory Comput. **11**, 5665 (2015), [2] F. Caruso, M. Dauth, M. J. van Setten, and P. Rinke, J. Chem. Theory Comput. **12**, 5076 (2016), [3] M. Dauth, F. Caruso, S. Kümmel, and P. Rinke, Phys. Rev. B **93**, 121115(R) (2016).

MM 13.4 Mon 16:00 GER 38

Addressing electron-hole correlation in core excitations of solids: A first-principles all-electron approach based on many-body perturbation theory — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In the framework of an all-electron implementation of many-body perturbation theory, we investigate K, L$_{2,3}$, and M$_4$ absorption edges of three exemplary solids, spanning a broad range of transition energies from a few hundred to several thousands eV. We find that transitions from deep core states, such as the Ti 1s states in TiO$_2$ and the Pb 3d states in PbI$_2$, are ruled by the long-range electron-hole attraction. Spin-orbit coupling and local fields play only a minor role for these excitations, which occur at several keV. The exchange interaction between the excited electron and the core hole becomes more relevant for smaller transition energies, as exemplified with the Ca L$_{2,3}$ edge in CaO. The overlap between Ca 2p and 3d states calls for a careful treatment of local field effects in order to describe these excitations. Our results, in good agreement with the available experimental data, are thoughtfully analyzed with advanced visualization tools in order to further gain insight into the electronic contributions and the spatial extension of the resulting electron-hole pairs.

MM 13.5 Mon 16:15 GER 38

Non-linear-screening contributions to photoemission spectra — •Marilena Tzavala[1,2], Claudia Rödl[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The state-of-the-art approach to calculate photoemission spectra of a broad range of materials is many-body perturbation theory in the GW approximation, sometimes combined with a cumulant expansion. The effective interaction that appears in these approaches is screened within the linear-response approximation. However, the photoemission of a core electron or a localized valence electron may be a strong perturbation, which suggests that non-linear screening effects could be important. We propose a formulation of the functional relations between the one-body Green's function and the screened interaction which is an alternative to Hedin's equations and which explicitly displays non-linear screening. Using a simple model, we show that exchange-correlation contributions are crucial in order to capture the non-linear effects. We also discuss how to apply the scheme to real materials using time-dependent density-functional theory (TDDFT).

MM 13.6 Mon 16:30 GER 38

Dynamic LDA for electronic excitations — •Marco Vanzini[1,2], Matteo Gatti[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Synchrotron SOLEIL, L'Orme des Merisiers, BP 48 Saint-Aubin, 91192 Gif sur Yvette, France

Density Functional Theory is an extremely useful tool for dealing with ground state properties such as the density or total energy. Kohn–Sham eigenvalues are often considered as approximated electronic excitations, but the resulting spectra are poor.

We propose a generalization of the Kohn–Sham approach to address in an exact framework electron addition and removal spectra. They can be measured by photoemission experiments, and can be evaluated using a computationally expensive non–local Self Energy. Our method is instead based on a frequency–dependent *local* potential [1], which significantly reduces the computing time of an ab–initio calculation.

To find this spectral potential in practice, we propose a jellium–based *dynamical* local density approximation (dynLDA): it relates the unknown potential to its homogeneous counterpart, via a non–trivial connector in space and frequency, which is based on physical insight.

In this talk, I will discuss the achievements and the limits of dynLDA, using models and real solids.

[1] M. Gatti et al., Phys. Rev. Lett. **99**, 057401 (2007).

MM 13.7 Mon 16:45 GER 38

Recent developments of the Sternheimer-GW method — •Martin Schlipf[1], Henry Lambert[1,2], and Feliciano Giustino[1] — [1]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom

The GW many-body perturbation method is an important tool to access accurate band gaps from first principles calculations. The conventional implementation determines the Green's function and the screened Coulomb interaction by a summation over unoccupied states tedious to converge. Giustino et al. demonstrated an alternative method to obtain these quantities by solving Sternheimer linear response equations. In this poster, we present our Sternheimer-GW software implemented in the Quantum Espresso framework and highlight some recent advances regarding the precision and stability of the method. We present our results for a small set of semiconducting materials and compare these to results obtained with conventional GW codes. We illustrate on selected examples the complete frequency dependent self energy, which is a natural product of the Sternheimer-GW method, and can be directly compared to experimental angle-resolved photoemission spectroscopy (ARPES) experiments.

MM 13.8 Mon 17:00 GER 38

Calculating electronic correlations in the CASTEP ab initio code — •Vincent Sacksteder[1] and Evgeny Plekhanov[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, — [2]Kings College London

We present new DMFT and GW features in the CASTEP DFT code. These features are designed to provide more accurate treatment of correlations between localized orbitals, of electronic screening, and of excited states. In present benchmarks on Cerium Oxide, the gamma phase of Cerium, and Silicon. We discuss the calculation of atomic forces within the GW framework.

MM 13.9 Mon 17:15 GER 38

Efficient G_0W_0 using localized basis sets: a benchmark for molecules — •Peter Koval[1,2], Mathias Per Ljungberg[1], and Daniel Sánchez Portal[1,2] — [1]Donostia International Physic Center, San Sebastian, Spain — [2]Centro de Fisica de Materiales, San Sebastian, Spain

Electronic structure calculations within Hedin's GW approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package [1], the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new G_0W_0 implementation based on a contour deformation technique to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set, using a pseudo-potential starting point provided by the popular density-functional package **SIESTA** [2]. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules [3] are compared to experiment and to reference all-electron calculations.

[1] `http://mbpt-domiprod.wikidot.com`; [2] Soler J. M., *etal* J. Phys.: Condens. Matter **14** (2002) 2745; [3] Knight J. W., *etal* J. Chem. Theory Comput., **12** (2016) 615.

MM 13.10 Mon 17:30 GER 38

A dynamic exchange correlation kernel derived from recent results for the homogeneous electron gas — •Martin Panholzer, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradies UMR 7642, CNRS-CEA/DSM, Ecole Polytechnique, Palaiseau, France

Time-Dependent Density Functional Theory (TDDFT) is a method of choice to calculate the dynamic structure factor of a wide range of materials. Even in the simplest Adiabatic Local Density Approximation (ALDA), plasmon spectra are generally well described. However, several shortcomings remain. In particular, the onset energy of the spectrum is underestimated [1], and dynamical effects such as lifetime damping and double plasmon excitations are absent [2].

In this work we investigate recent results for the dynamic response of the homogeneous electron gas (HEG)[3] to extract an exchange correlation kernel for TDDFT. In order to get an estimate of the validity of such an approach we compare our results for the dynamic kernel $f_{xc}(q,\omega)$ for the HEG with different kernels and known exact properties. We implemented this kernel with the simplest connection between the HEG and the real material, the mean density approximation. We compare results on simple metals, such as Na and Al, with experiments and ALDA. In order to explore the validity of such an approach we also applied the kernel to Si.

[1] G. Onida et al., Rev. Mod. Phys. 74, 601 (2002)
[2] M. Cazzaniga et al., Phys. Rev. B 84, 075109 (2011)
[3] H. M. Böhm et al., Phys. Rev. B 82, 224505 (2010)

MM 13.11 Mon 17:45 GER 38

Benchmark calculations of the electronic structure for molecules from the second-Born self-energy — •Michael Schüler[1] and Yaroslav Pavlyukh[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany

The non-equilbrium Green's function (NEGF) formalism provides a state-of-the-art tool for modeling modern spectroscopic experiments. In particular, time-dependent problems can be treated based on the Kadanoff-Baym equations. The underlying approximation to the self-energy has to be consistent with the treatment of the initial state - as captured by the Matsubara formalism - in order to guarentee the basic conservation laws. One of simplest non-trivial approximation to the self-energy is the second-Born approximation (2BA), which has been employed in numerous time-dependent studies. Systematic tests on the accuracy of the 2BA for various molecules has, however, been lacking so far. In our contribution we fill this gap by benchmark calculations for the 2BA for small molecules from the well established G2 test set. We demonstrate that the accuracy of the 2BA for predicting ionization potentials and electron affinities can compete with accurate quantum chemistry methods such as the Møller-Plesset perturbation theory and the coupled-cluster method. We also apply our method to a class of larger molecules, the diamonoids, which are in the focus of recent experiments and theoretical studies.

MM 13.12 Mon 18:00 GER 38

Performance of the GW approximation at reproducing key features in exact Kohn-Sham potentials — •Jack Wetherell[1], Leopold Talirz[1], Matt Hodgson[2], and Rex Godby[1] — [1]University of York, York, United Kingdom — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

One of the major goals of the GW method is to improve the accuracy of charge densities produced by density functional theory (DFT). In this work we test the applicability of one-shot GW from various DFT starting Kohn-Sham orbitals. Also we implement and test the fully self-consistent GW method. We test the applicability of these methods by using them to compute densities for simple model 1D systems from which the exact density can be obtained by the direct solution of the Schrodinger Equation. We choose a set of test systems that are either dominated by exchange or correlation, or contain non-local steps in the exact exchange-correlation potential. Also we analyse systems dominated by electronic interaction. We can also investigate how accurate the exchange-correlation potentials associated with the GW densities are, using our reverse-engineering algorithm.

MM 14: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Electro- and mechno-chemical coupling

Time: Monday 15:45–17:15 Location: BAR 205

MM 14.1 Mon 15:45 BAR 205

Electrocapillary coupling at metal surfaces from first principles — •Anja Michl[1], Jörg Weissmüller[2,3], and Stefan Müller[1] — [1]Hamburg University of Technology, Institute of Advanced Ceramics — [2]Hamburg University of Technology, Institute of Materials Physics and Technology — [3]Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics

The surface stress f of metallic surfaces reacts sensitively to excess charge q. This response can be characterized by the electrocapillary coupling parameter $\varsigma = \mathrm{d}f/\mathrm{d}q$. Due to their high surface-to-volume ratio, nanoporous metals respond with a macroscopic deformation to electric charging in electrolyte, which makes these materials interesting alternatives to conventional actuators. Exploiting a Maxwell relation, we have determined ς in terms of the response of the work function to in-plane strain for several metal surfaces, focusing mainly on the response of sp-bonded metals. It is found that aluminum surfaces exhibit positive coupling coefficients, whereas the other sp-bonded metals show the usual negative sign known from previous experimental and theoretical studies of clean transition metal surfaces. In addition, we investigate the impact of excess charge on surface structure and bonding via ab-initio simulation of metal surfaces in an external electric field in order to gain further insight into the underlying mechanisms. Both the direct effect on the surface stress via charging of the bonds and the indirect effect resulting from the charge-induced relaxation will be analyzed and discussed in relation to the trends of the determined coupling coefficients.

MM 14.2 Mon 16:00 BAR 205

Curvature induced stress and phase-boundary diffusion — •Raphael Schiedung, Reza Kamachali, Ingo Steinbach, and Fathollah Varnik — Ruhr Universität Bochum, Interdisciplinary Centre For Advanced Materials Simulations, Bochum, Deutschland

The multi-phase-field approach is generalized to treat diffusion, driven by mean curvature, parallel to surfaces between a condensed phase and its vapor as well as diffusion parallel to boundaries between condensed phases, 'phase-boundary diffusion'. Additionally, we present a treatment of surface-tension/energy for elastic bodies within the multi phase-field framework. The model is validated against the Young-Laplace law for the pressure gradient across the interface of spherical bodies and the prediction of Neumann's triangle relation for the force equilibrium at triple junctions. It is applied to thermal grooving and to the solid state sintering process of two spheres.

MM 14.3 Mon 16:15 BAR 205

Grain boundary diffusion of ions and electrons through a film or scale — •Markus Tautschnig, Nicholas Harrison, and Michael Finnis — Imperial College London, London SW7 2AZ, UK

A model for ionic and electronic grain boundary transport through thin films, scales or membranes with columnar grain structure is introduced. The grain structure is idealized as a lattice of identical hexagonal cells - a honeycomb pattern. Reactions with the environment constitute the boundary conditions and drive the transport between the surfaces. Time-dependent simulations solving the Poisson equation self-consistently with the Nernst-Planck flux equations for the mobile species are performed. The model is used to interpret alumina membrane oxygen permeation experiments. The simulation results provide a complete description of the measurements and insight into the microscopic processes underpinning the oxygen permeation of the membrane. Most notably, the hypothesized transition between p-type and n-type ionic conductivity of the alumina grain boundaries as a function of the applied oxygen gas pressure is observed in the simulations. The range of validity of a simple analytic model for the oxygen permeation rate, similar to the Wagner theory of metal oxidation, is quantified by comparison to the numeric simulations. The coupling between the defect fluxes and the stress state at the grain boundaries is discussed. The three-dimensional model we develop here is readily adaptable to problems such as transport in a solid state electrode, or corrosion scale growth.

MM 14.4 Mon 16:30 BAR 205

Oxygen adsorption on strained transition metal surfaces: An ab initio study of mechano-chemical coupling — •Gregor Feldbauer, Anja Michl, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Germany

Mechanical deformation can affect the adsorption and reaction processes of reactants on surfaces. Thus, by straining catalytically active surfaces their reactivity as well as selectivity can be influenced, which is of high importance, for example, in the field of heterogeneous catalysis. Here, transition metal surfaces, like Pd(111) and Ir(111), interacting with atomic oxygen are used as model systems. At first, the adsorption characteristics, e.g. the energetics, are investigated within the framework of density functional theory (DFT). The most favourable adsorption configurations are identified via the cluster expansion approach using DFT input data. Secondly, for various favourable oxygen configurations at the transition metal surfaces biaxial strain is applied in the surface plane to obtain the response of the adsorption energetics. Particularly, the coupling parameter between strain and adsorption energies is of interest to allow for a comparison with experiments. The coupling parameter is affected by the oxygen coverage as well as the occurrence of oxygen incorporation.

MM 14.5 Mon 16:45 BAR 205

Electrical modulation of the Poisson's ratio of nanoporous metals — •Lukas Lührs[1], Birthe Müller[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Nanoporous metals exhibit significant surface induced property modifications that are rendered possible by their large surface area to volume ratio. Among these materials nanoporous gold (NPG) appears an ideal model material due its high chemical stability and tunable surface area. Owing to its decisive electro mechanical coupling, electrical modulation of the strength and flow stress, elastic modulus, creep behavior and crack propagation have been demonstrated. However, the reliance of the lateral deformation behavior of NPG towards electrical tuning remains unclear.

In this contribution we study the influence of electrical modulation on the transverse mechanical coupling of NPG by the investigation of a metal/electrolyte hybrid material. We present experiments of NPG under compression testing in 1 M $HClO_4$ while varying the applied electrical potential, E. Our results show considerable changes of the plastic Poisson's ratio, ν_P, with E. We link these findings to the surface tension, γ, a capillary force that promotes a tension/compression asymmetry in the material. As γ depends on E, we show that the plastic lateral expansion behavior is governed by surface effects. In this line of argument we interpret the earlier reported ligament size dependence of ν_P.

MM 14.6 Mon 17:00 BAR 205

Size effects on hydrogen electrosorption in nanoporous Pd-Cu alloys — •Shan Shi[1,2], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg

Nanoporous (np) metals made by electrochemical dealloying exhibit a three dimensional metal network with high specific surface area, which couples the entire material behaviour to surface effects and specifically to electrocapillary effects that induce stress in the network. Electrochemical hydrogen electrosorption into bulk and surface of np-palladium-copper (np-PdCu) alloys results in reversible macroscopic expansion/contraction which can be monitored by in-situ dilatometry. This has been demonstrated to be an actuation mechanism and will be used to study the thermodynamics of the Pd-Cu-H system. Here, we fabricated mm-sized homogeneous monolithic np-PdCu samples by electrochemical dealloying. By thermal annealing after the synthesis, the characteristic ligament size was adjusted between 10 nm and 300 nm. Then we explored the influence of ligament size on both actuation performances (response time and strain amplitude) and thermodynamics (hydrogen solubility and hysteresis).

MM 15: Symposium SYLI: Interfacial Challenges in Solid-State Li Ion Batteries - Interface-dominated behaviour

Time: Monday 15:45–16:45 Location: IFW A

MM 15.1 Mon 15:45 IFW A

Interfacial double layers in all-solid-state Li-ion batteries: theoretical insights — •Johannes Voss[1], Saskia Stegmaier[2], Karsten Reuter[3], and Alan Luntz[1,2] — [1]SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [2]Stanford University, Stanford, CA, USA — [3]Technische Universität München, Germany

Neglecting potential electrochemical and mechanical stability issues of the interface between battery electrode and solid Li-ion conducting electrolyte, we present a theoretical study of charge double layers at ideal solid-solid interfaces. Based on DFT calculations for Li_3OCl, we discuss ionic charge carrier stabilities and interactions in the bulk and at interfaces to electrodes. We furthermore employ continuum models parametrized with DFT energies to understand charging at both the anode and cathode interfaces, respectively, and discuss how spacer materials could mitigate related potential interfacial issues.

MM 15.2 Mon 16:00 IFW A

Separation of Intra Grain and Grain Boundary Processes in Solid Electrolytes by High-Resolution Impedance Spectroscopy — •Andreas Mertens, Shicheng Yu, Deniz Guenduez, Hermann Tempel, Roland Schierholz, Hans Kungl, Rüdiger-A. Eichel, and Josef Granwehr — Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, D-52425 Jülich, Germany

Solid electrolytes are intensively researched for the next generation lithium-ion batteries. Yet their ion transport mechanisms must be better understood to improve their still too low ionic conductivity. Especially distinguishing between contributions from intra grain and grain boundary processes proved to be particularly challenging. This is mainly due to similar time constants of both processes at room temperature, leading to a strong overlap of their impedance contributions.

In this work we use a distribution of relaxation times analysis (DRT) in two dimensions (2D-DRT) to increase the resolution of impedance data measured at Li1.3Al0.3Ti1.7(PO4)3 (LATP) solid electrolyte samples sintered between 950°C and 1100°C. The second dimension of the 2D-DRT is given by data measured at varying temperatures between 10°C and 50°C. With the 2D-DRT it is possible to quantify the resistances and thus the activation energies of the intra grain and the grain boundary ionic charge transport processes under realistic battery operation conditions. Moreover, the ionic conductivity within the grain and the grain boundary could be determined.

MM 15.3 Mon 16:15 IFW A

Microstructural Properties of Li1.3Al0.3Ti1.7(PO4)3 Solid-

State Electrolyte — •Deniz Cihan Gunduz[1,2], Roland Schierholz[1], Shicheng Yu[1,2], Andreas Mertens[1,2], Hermann Tempel[1], Hans Kungl[1], and Rüdiger-A Eichel[1,2,3] — [1]Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, 52425 Jülich, Germany — [2]RWTH Aachen University, Institute of Physical Chemistry, 52074 Aachen, Germany — [3]Jülich-Aachen Research Alliance, Section JARA-Energy, Germany

Lithium-ion batteries are important in daily life. One task is to replace liquid electrolytes by solid ones and Li1.3Al0.3Ti1.7(PO4)3 (LATP) is a promising candidate exhibiting high ionic conductivities. For further development it is important to understand the influence of the microstructure on the ionic conductivity. Solid state electrolytes have been mainly investigated via means of electron microscopy (Scanning Electron Microscopy as well as Transmission Electron Microscopy). Here we combine these techniques with Laser Scanning Microscopy (LSM) to study the microstructure, such as grain size, grain boundary width, porosity and secondary phase content and distribution of LATP pellets sintered at different temperatures; and draw a relation to impedance measured on these pellets.

MM 15.4 Mon 16:30 IFW A

Development of Bulk-type All-Solid-State Lithium-ion Battery Based on Phosphate Backbone Materials — •Shicheng Yu, Hermann Tempel, Andreas Mertens, Deniz Cihan Gunduz, Svenja Benning, Roland Schierholz, Florian Hausen, Hans Kungl, and Rüdiger-A Eichel — Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, D-52425 Jülich, Germany

Considerable efforts have been devoted to the development of thick-film solid-state batteries while less achievement has been published owing to the poor interfacial compatibility between electrodes and electrolytes as well as low lithium ion transfer kinetics in solid materials. Here, we demonstrate the fabrication and performance of thick-film monolithic all-phosphate ceramic solid-state Li-ion batteries with high power density and cycling stability at ambient temperature based on LiTi2(PO4)3/C//Li1.3Al0.3Ti1.7(PO4)3//Li3V2(PO4)3/C. Theoretically, due to the crystal structure matchup of LiTi2(PO4)3, Li1.3Al0.3Ti1.7(PO4)3 and Li3V2(PO4)3, the solid-solid interface between Li1.3Al0.3Ti1.7(PO4)3 electrolyte and LiTi2(PO4)3 anode is expected to facilitate smooth contact while partially matched on the other side for the solid-solid contact of solid electrolyte and Li3V2(PO4)3 cathode. Besides, the operation voltage of the electrode pair is highly matched with the electrochemical window of solid electrolyte. Excitingly, by optimizing the morphology of electrode materials and composition of each layer, the all-solid-state lithium-ion battery, which has a controllable thickness from 0.7 up to 2 mm, showed high capacity and more than 300 stable cycles.

MM 16: Computational Materials Modelling - Novel Materials

Time: Monday 15:45–16:45 Location: IFW B

MM 16.1 Mon 15:45 IFW B

Ab initio derived phase stabilities for the design of novel Ce-based hard-magnetic materials — •Halil ibrahim Sözen, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Due to the developments in electrical transportation and renewable energies, hard magnetic materials composed of rare earths (RE) and transition metals (TM) have gained increasing importance in the last decades. Recently, there are attempts to develop alternative hard magnetic materials, RE-TM-X (X=Ti, W, Mo, Si, Al), that lift the dependence on a small number of RE elements. In order to support the efforts to find alternative materials concepts for hard magnetic applications, we performed ab initio calculations of finite temperature phase stabilities of Ce-based alloys. The Helmholtz free energy F(T,V) is calculated for all relevant competing phases using a sophisticated set of methods capturing vibrational, electronic, magnetic and configurational entropy contributions. The study includes unary Ce, binaries of Ce-Fe and Fe-Ti phases, and ternary Ce-Fe-Ti phases, for which the performance of our approach for rare-earth metals is tested. We observe that the presence of the CeFe2 phase retards any formation of promising Ce-Fe-Ti alloys. The study has therefore been extended to the impact of fourth alloying elements such as Cu and La, in order to provide strategies to solve this challenge.

MM 16.2 Mon 16:00 IFW B

Possible Gating on the Surface of a Weak Topological Insulator: Bi14Rh3I9 — •Madhav Prasad Ghimire[1] and Manuel Richter[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dresden Center for Computational Materials Science, DCMS, TU Dresden,D-01069 Dresden, Germany

Recently synthesized Bi14Rh3I9 was predicted to be a weak topological insulator. Scanning tunneling microscopy confirms this with a signatures of one-dimensional conducting states in the band gap at step edges of [(Bi4Rh)3I]2+ (2DTI) surface layers. However, the surface-layer gap is found 0.25 eV below the Fermi level (EF). Transport experiments are expected to be biased by intrinsic n-doping at the surface. Using density functional theory slab calculations we resolve this issue to shift EF into the surface layer gap without losing its topological properties. We perform chemical modification on the surface of Bi14Rh3I9: sparse layer of Iodine atoms is added onto the 2DTI surface. Investigation shows that deposition of one I atom per surface unit cell onto 2DTI surface opens a surface gap of 0.1 eV at EF, if simultaneously one I atom is removed from the dorsal spacer layer. The same effect with reduced gap size (0.08 eV) is observed for adding/removing I atoms in two fold higher concentration. Comparing our results with the experiment [ACS Nano, 2016] we predict that Fermi level can be shifted to the surface gap by deposition of I atoms onto the 2DTI surface in an appropriate range of concentration.

MM 16.3 Mon 16:15 IFW B

High Throughput searching for new topological materials — •Zeying Zhang[1,2], Yugui Yao[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China

The bottleneck of current studies on topological insulators is to identify better materials which can be fabricated into devices more feasibly. To search for novel topological materials, we developed a high throughput framework which can be utilized to screen over compounds with known crystal structures. We have applied our methods to ternary compounds of Bi and nitrides, with crystal structures obtained from Materials Project. For the moment, we focus on systems with small band gaps and with time-reversal symmetry. To characterize the topological properties including the surface states and topological invariants, the Wannier functions are constructed in an automated manner using a {\it poor-man's} algorithm, where the partial density of state from the first principles calculations is integrated in order to determine the proper projections and the energy windows. For the materials with inversion symmetry, we can easily get the topological invariants by counting the number of occupied states with odd parities. Till now, we have found two new topological compounds, and will discuss their topological properties in detail.

MM 16.4 Mon 16:30 IFW B

Charge transport in organic semiconductors: Towards an ACKS2-based polarizable force field — •Patrick Gütlein[1], Lucas Lang[1], Karsten Reuter[1], Jochen Blumberger[1,2], and Harald Oberhofer[1] — [1]Technische Universität München, Germany — [2]University College London, UK

Charge carrier transport, an integral part of diverse reactions and devices, is generally subject to the response of the surrounding environment. Especially in organic semiconductors the accurate theoretical treatment of the electronic rearrangements in the medium is a complex task. The high anisotropy and comparatively low dielectric screening require system sizes that challenge even efficient first-principles approaches like density-functional theory (DFT). In this situation the recently proposed atom-condensed Kohn-Sham density functional theory approximated to second order (ACKS2) approach[1] could represent a computationally undemanding, yet accurate alternative. In this approach, the linear response of the electron density and Kohn-Sham potential are captured by an atom-centered series expansion up to second order. For a range of molecular model systems we systematically compute the ACKS2 parameters with DFT and analyze their dependence on the intra-molecular degrees of freedom. We show that parts of the ACKS2 response can be approximated analytically, with the remaining parameters not varying strongly with respect to molecular motion. This represents an important first step in making ACKS2 applicable as a polarizable force field. [1] T. Verstraelen *et al.*, J. Chem. Phys. **138**, 7 (2013); *ibid* **141**, 19 (2014).

MM 17: Functional Materials I

Time: Monday 15:45–17:00 Location: IFW D

MM 17.1 Mon 15:45 IFW D

Fabrication of perovskite nano-rods in nanoporous anodic-aluminum oxide and their light harvesting characteristics — •Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Anodic-aluminum oxide (AAO) membranes consist of a highly ordered uniform hexagonal pore arrangement with pore diameters from $\sim$10 to $\sim$200 nm, and a thickness between $\sim$10 nm and $>$100 μm [1]. AAO membranes are comparably cheap and easy to synthesize, thus excellent for the synthesis of quasi-one-dimensional nano-rods.
Organometal-trihalide perovskites are organo-metal salts which are used as sensitizer in dye-sensitized solar-cells and as a light harvester in solid-state thin-film perovskite solar-cells,
with efficiencies up to $\sim$20 % [2].
The aim of this work is the fabrication of light harvesting devices, consisting of an ordered array of perovskite nano-rods that operate as quasi-one-dimensional perovskite solar-cells in parallel circuit. The nano-scaled confinement should result in preferred direction for charge carrier transport. Deposition conditions and resulting structures are studied, applying co-evaporation or precipitation from a highly concentrated perovskite solution. Optimum process parameters leading to a maximum filling of the AAO are deduced.
References:
[1] Y. Lei, W. Cai, G. Wilde, Prog. Mater Sci. 52 (2007) 465-539
[2] H. Snaith, J. Phys. Chem. Lett. 2013, 4, 3623-3630

MM 17.2 Mon 16:00 IFW D

Fabrications of Nanoporous Film and Nanowire Arrays with High Gas-Sensing Performances — •Shipu Xu, Huaping Zhao, Rui Xu, Liaoyong Wen, and Yong Lei — Institute of Physics & Institute of Micro- and Nanotechnologies (ZIK MacroNano), Ilmenau University of Technology, 98693 Ilmenau, Germany

Gas sensing has an important effect on many aspects in our society, and has gained much progress by nanostructuring materials. Herein, nanoporous film and nanowire arrays were respectively fabricated on the device substrate and directly used as the sensing platform. Different kinds of N- and P-type sensing materials (e. g., SnO2, Fe2O3 and NiO) were independent or composited with graphene to serve as functional materials. Given by the intrinsic advantages of nanostructuring (e. g., large specific area and rich active sites), as-prepared sensors had exhibited high-sensitive and rapid sensing response in the ambient atmosphere even at room temperature. Furthermore, the pristine sensing property could be manipulated by their nanostructures, such as surface pore size of porous film or the length of nanowire arrays, to meet the requirements of the practical applications. Obviously, the way to improve and manipulate the sensing property that based on the nanostructuring (e. g., nanoporous film and nanowire arrays) enables the feasibility of next-generation gas-sensor.

MM 17.3 Mon 16:15 IFW D

Compact Nanowire Sensors Probe Microdroplets — Julian Schütt[1], Bergoi Ibarlucea[1,2], Rico Illing[1,2], Felix Zoergiebel[1,2], Sebastian Pregl[1,2], Daijiro Nozaki[1], Walter Weber[2,3], Thomas Mikolajick[2,3], Larysa Baraban[1,2], and •Gianaurelio Cuniberti[1,2] — [1]Max Bergmann Center of Biomaterials and Institute for Materials Science, Dresden — [2]Center for Advancing Electronics Dresden — [3]Namlab GmbH, Dresden

Here we demonstrate a first combination of droplets microfluidics with the compact silicon nanowire field effect transistor (SiNW FET) in the microfluidic channel for in flow electrical detection of aqueous reactor-drops. Apart from detection events, we chemically probe the content of numerous droplets in a row as independent events (up to 10^4), and resolve the pH values and ionic strength of the solution, resulted in a change of a source-drain current ISD through the nanowires. We demonstrate the capability of the novel droplets based nanowire platform for bioassay applications and carry out a glucose oxidase (GOx) enzymatic test for glucose detection. Optic-less and noninvasive measurements of these parameters in aqueous droplets have a great impact on the area of biodetection and bioanalytics as a HTS tool for pathogens, drug assays, and evaluation of the enzymatic activities.

MM 17.4 Mon 16:30 IFW D

Multiplexing of imperceptible temperature sensor arrays for on-skin applications — •Tetiana Voitsekhivska, Jürgen Fassbender, and Denys Makarov — Helmholtz-Zentrum-Dresden-Rossendorf e.V., Dresden, Germany

Beside the direct temperature measurement resembling the standard health indicator, the access to the body core temperature and its temporal variations provides the information, which is absolutely crucial to assess the psycho-physiological conditions of the patient, e.g. level of stress. To measure spatial and temporal temperature gradients, multiple temperature sensors have to be attached and processed on the human body surface [1, 2].

Here, we introduce a thermal characterization technology for real - time monitoring the human body temperature using arrays of highly compliant on-skin temperature sensors, realized on 6-micrometer-thick polymeric foils, which are haptically not perceived when worn on the skin. Beside the realization of the arrays of imperceptible temperature sensors, we put strong emphasis on the integration of a multiplexing unit on flexible foils in order to achieve measurements with mapping capabilities.

[1] R. Chad Webb et al., *Nature Materials* **12**, pp. 938-944 (2013).
[2] Tomoyuki Yokota et al., *PNAS* **112**, pp. 14533-14538 (2015).

MM 17.5 Mon 16:45 IFW D

Diamondoid-based materials for sensors, nanopores, and molecular devices — Bibek Adhikari[1], Ganesh Sivaraman[1], Frank C. Maier[1], Rodrigo G. Amorim[2,3], Ralph H. Scheicher[2], Sheng Meng[4], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden — [3]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [4]Institute of Physics, Chinese Academy of Sciences, Beijing, China

Diamondoids are tiny hydrogen-terminated diamond-like cages which can assume a variety of sizes, have tunable optoelectronic properties, and can be selectively modified. Based on these properties, we investigate the used of diamondoids as functionalization molecules. First, we prove that small diamondoids can form measurable hydrogen bonds to small molecules, such as DNA nucleobases and can render nanopores highly biosensitive. We next investigate different molecular anchors, thiols and carbene molecules, to functionalize metal surfaces, with a prospect to use these in field emitting devices. We extend this study by examining diamondoid-based molecular break-junctions and link their efficiency to their exact microstructure and the relevant experimental conditions. Our investigations are based on quantum-mechanical calculations together with the non-equilibrium Green's functions formalism and the evaluation of the electronic and quantum transport properties of the diamondoid-based materials. We discuss the relevance of our results in using diamondoids in novel applications.

MM 18: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Experimental Characterization

Time: Monday 17:30–18:45 Location: BAR 205

Topical Talk MM 18.1 Mon 17:30 BAR 205

Experimental investigations on the relationship between crystallographic character of grain boundaries and their functional and mechanical properties in various engineering materials. — •Stefan Zaefferer, Dayong An, Zhangqi Wang, Fady Archie, and Guillaume Stechmann — Max-Planck-Institut für Eisenforschung

Grain boundaries are important defects in crystalline solids because they influence a large number of properties, like strength of ductile materials, fracture resistance and corrosion resistance of various metals, or efficiency losses in polycrystalline solar cells. The exact correspondence between the properties and the crystallographic nature of grain boundaries is in many cases not well understood which is mainly due to the fact that grain boundaries are characterized by 8 degrees of freedom, namely 5 rotational parameters and 3 translational ones. The translational parameters are very difficult to measure and it is not clear whether they are independent of the others. The rotational parameters, that is the grain boundary misorientation (3 parameters) and the grain boundary plane, can however be measured using 3D or pseudo-3D orientation microscopy. With these techniques we are able to study the influence of all parameters on grain boundary properties. In the presentation we will introduce the various techniques and show application examples. In particular we will present results on the corrosion of grain boundaries of austenitic stainless steels in aqueous acid solutions and in salt melts, on fracture resistance in DP steels and on the influence on the performance of CdTe solar cells.

MM 18.2 Mon 18:00 BAR 205

Mechanical Testing of Copper Alloy Micropillars Containing a Twin Boundary — •Sebastian Krauss, Jan Philipp Liebig, Mathias Göken, and Benoit Merle — Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

Nanotwinned metals are a promising class of modern materials combining a very high strength with a high ductility and excellent electrical properties. This remarkable strength is connected to the very good efficiency of twin boundaries as obstacles to dislocation motion. In order to further characterize these interactions, micropillars containing single twin boundaries with different orientations were compressed with a flat punch, and subsequently investigated in the scanning electron microscope. The investigations concentrated on copper and α-brass, which is a low stacking-fault energy alloy exhibiting a high density of recrystallization twins. Coherent twin boundaries were selected from an EBSD orientation mapping of the sample and oriented by means of a custom sample holder. FIB-milling at these interfaces provided micropillar samples containing a single twin boundary. Single crystalline reference samples were obtained from the bulk of the grain located on both sides of the twin boundary. The microcompression tests allowed quantifying the influence of the twin boundary barrier on the strength of the sample. The activated glide systems were subsequently identified from slip trace analysis and STEM mapping of lamellas obtained by lift-off from the bulk of the tested micropillars.

MM 18.3 Mon 18:15 BAR 205

Interface Nanolayer Analysis in Al-Cu FSW Lap Joints — •Roland Marstatt[1], Markus Krutzlinger[2], Johannes Luderschmid[1], Ferdinand Haider[1] und Michael F. Zaeh[2] — [1]Chair for Experimental Physics 1, University of Augsburg, Universitaetsstraße 1, 86159 Augsburg, Germany — [2]Institute for Machine Tools and Industrial Management (iwb), Technical University of Munich, Boltzmannstraße 15, 85748 Garching, Germany

Friction Stir Welding (FSW) is a suitable technology to join dissimilar materials. The material does not exceed the solidus temperature during FSW and the heat effect is much lower compared to fusion welding processes. So FSW can produce high quality joints between dissimilar metals with a minimum of deleterious intermetallic phases. Interfacial phases can cause embrittlement, but also lower the electrical and thermal conductivity through the interface. While intermetallic nanometer scaled layers in friction stir welded dissimilar metal joints were mentioned in literature, the quantitative understanding of the correlation of process parameters and interface structure is still a subject of research. In this study, the formation and atomic structure of the nanometer scaled intermetallic layers at the bonding interface of aluminium copper lap joints were analysed. These layers play a key role for the joining mechanism. The thickness of an intermetallic layer highly depends on the process temperature, which can be controlled by the welding parameters. The obtained results lead to a better understanding of the correlations and therefore enable process control and predictability. *Supported by the DFG as part of SPP 1640.*

MM 18.4 Mon 18:30 BAR 205

Experimental determination of interface strength and toughness in multi-layered thin films — Ruth Konetschnik[1], Darjan Kozic[2], Ronald Schöngrundner[2], Hans-Peter Gänser[2], Roland Brunner[2], and •Daniel Kiener[1] — [1]Department Materials Physics, Montanuniversität Leoben, Austria — [2]Material Center Leoben Forschungs GmbH, Austria

In recent years, ongoing miniaturization has led to increasingly complex thin film combinations and geometries. As macroscale tests are not applicable, miniaturized tests are suggested to study the materials response in state of the art and future devices at small length scales. Here, we concentrate on the local determination of interface strength and toughness in layered thin films also taking into account the residual stresses. The materials investigated are sputter deposited Cu-W-Cu and W-Cu-W trilayer systems, with an individual layer thickness of 500 nm, on a Si substrate. Samples with different geometries such as notched bending beams, double cantilever beams, and miniaturized shear specimens are fabricated via cross section polishing and focused ion beam (FIB) milling to quantitatively test individual interfaces. Subsequently, miniaturized fracture experiments parallel and perpendicular to the interfaces are performed in-situ in the SEM to obtain comprehensive knowledge of the fracture and interface toughness. We emphasize the importance of elastic and plastic incompatibilities and residual stresses when addressing fracture mechanical quantities of multi-layered thin film systems and discuss challenges and benefits of our different approaches.

MM 19: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - sulphate- and phosphate-based electrolytes

Time: Monday 17:15–18:00 Location: IFW A

MM 19.1 Mon 17:15 IFW A

Aliovalent substitution in garnet type solid-state electrolytes for solid-state lithium-ion batteries — •Anja Paulus[1], Maike Wirtz[1], Sabrina Heuer[1], Peter Jakes[1], Hans Kungl[1], and Rüdiger Albert Eichel[1,2] — [1]Fundamental Electrochemistry (IEK-9), Institute of Energy and Climate Research, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]Institut für Physikalische Chemie (IPC), RWTH Aachen University, D-52074 Aachen, Germany

Conventional lithium-ion batteries consist of an electrolyte containing toxic, flammable organic liquids which lead to several safety issues such as leakage and burning of the battery. In order to overcome these safety issues solid-state electrolytes could be an alternative to obtain powerful lithium-ion batteries. The garnet type electrolyte Li7La3Zr2O12 shows promising properties in terms of high lithium-ion conductivity and a good stability against lithium. There are two modifications known for this material, on the one hand a tetragonal one which is thermodynamically stable at room temperature and on the other hand a cubic high temperature modification. The cubic structure shows a lithium conductivity of two orders of magnitude higher than the conductivity of the tetragonal one. One possibility to stabilize the cubic structure at room temperature or lower temperatures is by aliovalent substitution. Aluminum substitution on the lithium site shows a lithium conductivity of 3.41*10-4 S*cm-1 for Li6.4Al0.2La3Zr2O12 at room temperature [1]. Our focus is to study the influence of aliovalent substitution on the properties of garnet type solid-state electrolytes by various techniques. 1.C.Tsai et al., J. Electroceram., 2015, 35, 25-32.

MM 19.2 Mon 17:30 IFW A

Defect chemistry of solid electrolyte $Li_4P_2S_6$ by first-principles calculations — •Marcel Sadowski, Sabrina Sicolo, and Karsten Albe — Institute of Materials Science, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Glassy, glass-ceramic and crystalline lithium thiophosphates have attracted interest as solid electrolytes for all-solid-state batteries. Despite similar structural motifs, these materials exhibit a wide range of compositions, structures and ionic conductivities. For the glass-ceramic consisting of crystalline $Li_4P_2S_6$ and glassy $Li_4P_2S_7$, for example, contradictory ionic conductivities were reported. In this contribution we present density functional theory (DFT) calculations on the defect thermodynamics and kinetics of crystalline $Li_4P_2S_6$. [1] Despite the existence of low energy diffusion paths, the overall conductivity is inhibited by high defect formation energies. This supports the hypothesis that the conductivity of the $Li_4P_2S_7/Li_4P_2S_6$ composite material is determined by the relative amount of glassy and crystalline phases.

Furthermore, thermodynamics predict the instability of $Li_4P_2S_6$ against metallic lithium. Corresponding interface models for different surface terminations of $Li_4P_2S_6$ show the barrierless formation of an interphase reminiscent of Li_2S, which might act as a passivating layer and protect the electrolyte from further decomposition.

[1] C. Dietrich, M. Sadowski, S. Sicolo, D. A. Weber, S. J. Sedlmaier, K. S. Weldert, S. Indris, K. Albe, J. Janek, W. G. Zeier, Chem. Mater. DOI:*10.1021/acs.chemmater.6b04175 (2016).

MM 19.3 Mon 17:45 IFW A

Systematic Search for Lithium Ion Conducting Compounds by Screening of Compositions Combined with Atomistic Simulation — •Daniel Mutter[1,2], Daniel Urban[2], and Christian Elsässer[1,2] — [1]Freiburger Materialforschungszentrum (FMF), Albert-Ludwigs-Universität Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg — [2]Fraunhofer Institut für Werkstoffmechanik (IWM), Wöhlerstraße 11, 79108 Freiburg

Solid state electrolytes (SSEs) with high Li conductivity can significantly improve Li ion accumulators in terms of electrochemical efficiency, thermal and mechanical stability, and environmental compatibility, leading to an enhanced range of applications for these high energy density batteries. Compounds crystallizing in the structure of $NaZr_2(PO_4)_3$ (NZP) are regarded as promising SSEs, mainly because of their three-dimensional diffusion network enabling fast transport of Li ions through well defined channels. Starting from $LiTi_2(PO_4)_3$, we analyzed a large variety of NZP compounds by systematically screening the relevant parts of the periodic table, replacing atoms on the Ti and P sublattices by isovalent elements. The influence of these elemental substitutions on structural stability, preferred Li sites, ionic mobility, migration paths and diffusion mechanisms were analyzed by means of a combined approach of multiple computational methods with different levels of accuracy, ranging from static energy landscape and molecular dynamics simulations with ionic bond valence potentials to density functional theory calculations combined with the nudged elastic band method.

MM 20: Computational Materials Modelling - Defect structure and formation

Time: Monday 17:00–18:15 Location: IFW B

MM 20.1 Mon 17:00 IFW B

Prediction of Morphologies at Inorganic/Organic Interfaces with Machine Learning on the Example of TCNE/Cu(111) — •Michael Scherbela, Lukas Hörmann, Veronika Obersteiner, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Many properties of thin films, such as their solubility or conductivity, depend strongly on the crystal structure of the adsorbed molecules. A major step towards designing new materials is therefore understanding and predicting the polymorphs that form at interfaces. This could in principle be done by finding low energy structures using ab-initio methods. However, the many degrees of freedom lead to a rich polymorphism that prohibits an exhaustive search for the global minimum. We show on the example of Tetracyanoethylene/Cu(111) that this challenge can be tackled with a combination of coarse-graining and machine learning:

First we determine adsorption geometries that isolated molecules adopt on the substrate. We then build supercells by combining these isolated adsorption geometries to generate a set of possible "guess polymorphs". This discretizes the configurational space to a huge, but finite size. Using optimal design methods we select a small, representative subset, calculate its energies using DFT and extract effective interactions between adsorbates. This provides an efficient energy prediction for all remaining guess polymorphs which is exploited by sampling the energetically most promising structures and iterated relearning. For TCNE/Cu(111), we predict stable polymorphs for different coverages and explain an experimentally observed phase transition.

MM 20.2 Mon 17:15 IFW B

Ab-initio study of the interplay of hydrogen and microstructure in Ni-based superalloys — •Poulumi Dey, Zahra Tarzimoghadam, Dirk Ponge, Eunan McEniry, Tilmann Hickel, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Ni-based superalloys with their excellent corrosion resistance are attractive for applications where exposure to hydrogen is inevitable such as sour gas environments in oilfields. The adverse impact of hydrogen on the desired mechanical properties of these alloys, however, often restricts the acceptable strength levels of these materials. In the present work, we perform ab-initio calculations to establish the fact that the delicate behavior of hydrogen sensitively depends on microstructure features present in the superalloy. In particular, we consider the volume fractions of different precipitate phases which can be experimentally adjusted by annealing and aging conditions. With the aid of density functional theory (DFT), we perform a quantitative analysis of the hydrogen solution enthalpies within the precipitates and their interface to the matrix material. The study thus provides crucial information about the impact of chemistry and crystal structure on the hydrogen solubility and diffusivity at the interfaces as well as possible nucleation points for hydrogen-induced fracture in the material.

MM 20.3 Mon 17:30 IFW B

Embedded-atom study of low-energy equilibrium triple junction structures and energies — •Sebastian Eich and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

We present an atomistic study of the structures and defect energies of iron triple junctions (TJs) in polycrystalline materials. Line energies of bulk TJs (merging three grain boundaries (GBs)) and surface TJs (merging one grain boundary and two surfaces) are found to be very low. In absolute value, they amount to only a few 10^{-10} Jm^{-1}. Remarkably, defined as a correct excess energy relative to the GBs, the bulk TJ energy is determined to be negative in all studied configurations with an average value of -2.8×10^{-10} Jm^{-1}. These quantitative results are in contrast to various experimental attempts, but they fully agree with simple geometric estimates.

Finally, we relate the negative TJ line energies to the excess segregation at TJs in a realistic Fe–Cr model system.

[1]: S. Eich, G. Schmitz, Embedded-atom study of low-energy equilibrium triple junction structures and energies, Acta Mater. 109 (2016) 364–374.

[2]: S. Eich, D. Beinke, G. Schmitz, Embedded-atom potential for an accurate thermodynamic description of the iron–chromium system, Comput. Mater. Sci. 104 (2015) 185–192.

MM 20.4 Mon 17:45 IFW B

Heterogeneous nucleation at prestructured seeds in Ni — •Grisell Diaz Leines, Ralf Drautz, and Jutta Rogal — Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

The fundamental principles of crystallization and polymorph selection in metals are largely determined during the early stages of nucleation. The presence of impurities and the crystallization conditions influence directly the microstructural evolution of the material. In this work we investigate the influence of small prestructured seeds on the nucleation mechanism during solidification in nickel. We employ transition path sampling simulations to enable the investigation of nucleation on the atomistic level. The analysis of the transition path ensemble obtained from our simulations indicates that, in comparison to homogeneous nucleation the presence of fcc and hcp seeds enhances the nucleation rate and determines the structure of the growing nuclei. Icosahedral and bcc seeds on the other hand have no effect on either the mechanism or the nucleation rates. Furthermore, we demonstrate that different conditions of undercooling and pressure determine the amount of hcp and fcc coordinated atoms that compose the growing nuclei and therefore the selected polymorph. Our results provide atomistic insight into the process of seeded heterogeneous nucleation at different crystallization conditions and shed light on the principles of polymorph selection in Ni.

MM 20.5 Mon 18:00 IFW B

Electrons and phonons on equal footing: Band renormalization in Diamondoids — •Pablo Risueno, Peng Han, and Gabriel Bester — UHH, Grindelallee 117, Hamburg, Germany

Recent work on electron-phonon coupling has considered the renormalization of the electronic states due to the interaction with the vibronic degrees of freedom. The complementary effect that electrons have on phonons has been mostly ignored. In turn, these renormalized phonon energies have a renormalization effect on the electronic states, which calls for a self-consistent treatment of electrons and phonons, treating both on equal footing. We will show how this self-consistent effect can be incorporated into the calculations and quantify its importance. We show results for small carbon clusters known as diamondoids, which are relevant in technological applications and are computationally tractable by our numerical approach.

MM 21: Functional Materials II

Time: Monday 17:15–18:45 Location: IFW D

MM 21.1 Mon 17:15 IFW D

Hydrogen induced defects in the palladium/rutile titanium dioxide model system — •Marian David Bongers[1], Mohsen Sotoudeh[2], Vladimir Roddatis[1], Jakub Čížek[3], Carsten Nowak[1], Martin Wenderoth[4], Peter Blöchl[2], and Astrid Pundt[1] — [1]Institut für Materialphysik, Univ. Göttingen — [2]Institute for Theoretical Physics, Clausthal Univ. of Technology — [3]Department of Low-temperature Physics, Charles Univ. in Prague, Czech Republic — [4]IV. Physikalischen Institut, Univ. Göttingen

The palladium (Pd)/titanium dioxide (TiO_2) system is used in a range of applications where in particular the interaction with hydrogen (H) is of interest. We use in-situ transmission electron microscopy (ETEM) and electron energy loss spectroscopy (EELS) on cross-sectional Pd/TiO_2 lamella focusing on the interface. The EELS studies show a small change of the Ti L edge signal in the 3 nm close vicinity of the interface, for hydrogen gas pressures of about 10^{-1} mbar. These small changes can be attributed to a shift in the density of states (DoS) by about 1 eV, by the presence of hydrogen. This is supported by projector augmented wave (PAW) code simulations using the local hybrid density functional PBE0r [1]. We suggest interstitial hydrogen to be the dominant hydrogen induced defect in bulk, while it is the oxygen-vacancy filled with hydrogen nearby the interface. These defects determine the corresponding Fermi level position in bulk and at the interface. This work is supported by the Deutsche Forschungsgemeinschaft via SFB1073, project C06 and C03 as well via the Heisenberg grant PU131/9-2. [1] M. Sotoudeh, M. Bongers, et al., submitted

MM 21.2 Mon 17:30 IFW D

Magnetocaloric properties of melt-spun NiCoMnAl Heusler ribbons — •Bruno Weise[1], Niclas Teichert[2], Andreas Becker[2], Lars Helmich[2], Maria Krautz[1], Andreas Hütten[2], and Anja Waske[1,3] — [1]IFW Dresden, Institute for Complex Materials, Dresden, Germany — [2]CSMD, Department of Physics, Bielefeld University, Bielefeld, Germany — [3]Institute of Materials Science, TU Dresden, Dresden, Germany

Within the group of magnetocaloric Heusler alloys NiCoMnAl is a promising alloy system for magnetic refrigeration. It is rare-earth free, non-toxic and none of the constituent elements is short on stock. In thin films of NiCoMnAl, an entropy change of up to $\Delta S = 17.5\ J/kgK$ for a magnetic field change of $\Delta\mu_0 H = 5\ T$ was observed [1], hence thin films can be used as a model system to test new materials. This subsequent study applies these results to bulk materials.

Samples of the nominal composition $Ni_{40}Co_{10}Mn_{30}Al_{20}$ have been produced by melt spinning to achieve near net shaped thin plates for the use in a refrigeration bed. The ribbons were annealed for up to 50 h and the structure was checked with XRD. With electron microscopy the microstructure of the ribbons was studied. An optimal heat treatment time for highest entropy change was found and the adiabatic temperature change for this annealing time was determined.

[1] N. Teichert et al., Phys. Rev. B 91, 184405 (2015).

MM 21.3 Mon 17:45 IFW D

In-situ dehydrogention and positron annihilation spectroscopy of Mg2Fe thin films — •Thu Trang Trinh[1,2], Marciej Oskar Liedke[2], Andreas Wagner[2], Rene Heller[2], Herman Schreuders[3], Bernard Dam[3], Kohta Asano[4], and Kay Potzger[2] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]Helmholz-Zentrum Dresden Rossendorf, 01328 Dresden, Germany — [3]Delft University of Technology, 2629HZ Delft, Netherlands — [4]AIST, Tsukuba 8565, Japan

Mg2Fe hydride belongs to the most promising candidates for application as light weight storage material in a future hydrogen economy. Recently, it has been shown that due to chemochromism, Mg2Fe is also a low-cost and rare-earth-free candidate for switchable mirrors upon hydrogen loading. However, the interaction between defects and hydrogen on the atomic scale remains not completely understood, despite the fact that the behaviour of hydrogen in metals is strongly affected by the presence of defects. Due to the positive binding energy between hydrogen and vacancy, the hydrogen atoms get trapped at existing defects which thus play an important role for the hydride formation.

We present a comparative and systematic study on the defects in Mg2Fe and their interaction with hydrogen by means of positron annihilation spectroscopy (PAS). We present first results of the temperature dependence of the open volume defects during annealing of Mg2FeH6 thin films, which was performed by an unique high vacuum system for defect manipulation and analysis (AIDA) at the positron beamline at the Helmholtz-Zentrum Dresden-Rossendorf.

MM 21.4 Mon 18:00 IFW D

Compliant on-skin compass for artificial magnetoception — •Gilbert Santiago Cañon Bermúdez, Jürgen Fassbender, and Denys Makarov — Helmholtz-Zentrum-Dresden-Rossendorf e.V., Dresden, Germany

Flexible electronics has inspired novel concepts like electronic skins[1] and more recently, magnetosensitive skins[2], i. e., artificial skins which allow humans to perceive magnetic fields. This ability to detect and respond to magnetic fields, commonly referred to as magnetoception, has sparked several legends since the old sailing times. Back then, it was believed that compass rose tattoos would allow sailors to always find the way home. Here, we present a flexible electronics platform to turn this ancient belief into a functional on-skin compass system. The highly compliant compass is prepared on 6-micron-thick polymeric foils and relies on the anisotropic magnetoresistance (AMR) effect in magnetic thin film sensors. Its response is tailored to be linear and possess maximum sensitivity around the earth's magnetic field by using a barber pole scheme, which forces the current in the sensor to flow 45 degrees skewed with respect to the easy axis of the AMR stripes. We envision that this on-skin compass could support research efforts on biomagnetic orientation and novel magnetic interactive devices. In the latter case, the applications span a plethora of tasks from virtual or augmented reality systems to touchless security systems and magnetic tags.

[1] D. H. Kim et al., Science 333, 838 (2011).

[2] M. Melzer et al., Nature Commun. 6, 6080 (2015).

MM 21.5 Mon 18:15 IFW D

Photoemission Spectrscopy of Type-II Weyl Semimetal Candidate MoTe2 — •Andrew Patton Weber[1,2], Nan Xu[1,2], Stefan Muff[1,2], Mauro Fanciulli[1,2], Arnaud Magrez[1], Phillipe Bugnon[1], Helmuth Berger[1], BQ Lv[3], Bin Bin Fu[2,3], Christian Matt[2], Joel Mesot[1,2,4], Hong Ding[3], Ming Shi[2], and Jan Hugo Dil[1,2] — [1]Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, Villigen-PSI, Switzerland — [3]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China — [4]Laboratory for Solid State Physics, ETH Zurich, Zurich, Switzerland

Topological matter can often be identified by signatures presented by the surface electron-structure. Type-II Weyl semimetal candidates, in which surface Fermi arcs can overlap with the projection of bulk Fermi pockets, have proven to be more difficult to characterize by these means, leading to controversies. The present work clarifies the situation for the case of the octahedral polytype of MoTe2 through temperature-dependent spin- and angle-resolved spectroscopy experiments. It is found that the appearance of large spin-polarized Fermi arcs (extending over more than 12% of a reciprocal lattice vector and exhibiting nearly full spin-polarization), occurs as a consequence of the transition from the inversion-symmetric 1T' structure to the inversion-symmetry-breaking Td structure. Moreover, helical spin-textures are found to be absent near the large Fermi arcs. These results indicate a topological origin for Fermi arc-like states.

MM 21.6 Mon 18:30 IFW D

Identifying detrimental effects for multi-band superconductivity - Application to $\mathbf{Sr_2RuO_4}$ — •Aline Ramires[1] and Manfred Sigrist[2] — [1]Institute for Theoretical Studies, ETH Zurich, 8092 Zurich, Switzerland — [2]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

We propose a general scheme to probe the compatibility of arbitrary pairing states with a given normal state Hamiltonian by the introduction of a concept called *superconducting fitness*. This quantity gives a direct measure of the suppression of the superconducting critical temperature in the presence of key symmetry-breaking fields. A merit of the superconducting fitness is that it can be used as a tool to identify nontrivial mechanisms to suppress superconductivity under various external influences, in particular, magnetic fields or distortions, even in complex multiorbital systems. In the light of this concept we analyze the multiband superconductor Sr_2RuO_4 and propose a new mechanism for the suppression of superconductivity in multiorbital systems, which we call interorbital effect, as a possible explanation for the unusual limiting feature observed in the upper critical field of this material.

MM 22: Poster session I

Time: Monday 19:00–20:00 Location: P4

MM 22.1 Mon 19:00 P4

Nano-scale grain substructure as a factor determining transport properties of ceramic manganites — •Anastasiia Novokhatska and Gennadiy Akimov — Donetsk Institute for Physics and Engineering named after A. A. Galkin of the National Academy of Sciences of Ukraine, Av. Nauky 46, Kyiv, 03680, Ukraine

We present a new method for obtaining nano-scale grain substructure in La0.65(Ca,Sr)0.35MnO3 manganite ceramics sintered at 1500 °C by means of excess manganese from 10 and 20 % as well as the study of its structure and magnetoresistive properties. With results of the scanning electron microscopy research, it is shown that the presence of excess manganese allows to sinter ceramics at temperatures of up to 1500 °C while maintaining the chemical and phase composition. The ceramic samples consist of manganite grains with sizes 100 μm and Mn3O4 hausmannite grains. Moreover, investigations of thermally etched cleaved surfaces of ceramics grains together with X-ray diffraction data showed that manganite grains have internal layered structure with the layer size of 70-140 nm where each layer is a perfect single crystal of manganite of the stoichiometric composition. It is found that the emergence of a nano-scale substructure of grains is accompanied by the resistivity drop (two orders of the magnitude) and by reduction of the slope of its temperature dependence. Moreover, the metal-insulator transition temperature is shifted towards a lower temperature and the value of the magnetoresistivity (at the applied magnetic field of 5 kOe) increase in 2.5 times.

MM 22.2 Mon 19:00 P4

Electrochemical studies on single particles of active electrode materials for lithium-ion batteries (LIBs) — •Markus Sebastian Friedrich[1], Simon Burkhardt[1], Limei Chen[1], Matthias Thomas Elm[1,2], and Peter Jens Klar[1] — [1]Heinrich-Buff-Ring 16, 35392 Giessen — [2]Heinrich-Buff-Ring 17, 35392 Giessen

Lithium intercalating and deintercalating materials such as $Li(Ni_xCo_yMn_{1-x-y})O_2$ (NCM) have been widely investigated. These materials are of interest for lithium-ion batteries due to their high theoretical capacity and high reversibility of the intercalation/deintercalation processes. Most of the studies were carried out on composite electrodes, which not only contain the pure NCM material, but also organic binder and conductive agents. These influence the electrochemical properties of the electrode significantly. To examine the influence of the active electrode material's structure on energy storage and energy conversion of a cell system, a deeper understanding of the intrinsic properties of single (active) particles is needed. Besides widely used microelectrode setups, we developed a technique to contact individual particles in an electrochemical cell and perform measurements like CVs and EIS techniques, to characterize the pristine NCM particles with focus on conductive properties. To prepare our samples we used photolithography for structuring a photoresist on an F_xSnO_2 (FTO) coated glass substrate, to form holes of well defined size to trap single particles of NCM.

MM 22.3 Mon 19:00 P4

Electrochemical properties of hierarchically structured C-coated $\mathbf{LiFe_xMn_{1-x}PO_4}$ — •Enzo Moretti[1], Christoph Neef[1], Elisa Thauer[1], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institut für Physik, Universität Heidelberg — [2]Centre for Advanced Materials, Universität Heidelberg

High-purity $LiFe_xMn_{1-x}PO_4$ with various doping levels $x = 0.1$ - 0.5, different carbon contents, and variable primary particles size have been synthesized by a combination of solid-state synthesis, optical floating zone treatment, and ball milling. The obtained nanosized materials were assembled to larger, i.e. micrometer-sized, hierarchically structured entities by thermal treatment and usage of different organic additives. Applicability of the resulting hierarchically structured product for cathodes in lithium-ion batteries is investigated by means of cyclic voltammetry and galvanostatic cycling. The effect of both the primary and secondary particle size and the carbon ratio is studied in particular. In parallel, the obtained doping series is used to study the evolution of antiferromagnetic order at low temperature as well as the average magnetic moment per metal ion, i.e. the mean electron configuration.

MM 22.4 Mon 19:00 P4

Design of Ti-based alloys with austenitic Ni-Ti nanoprecipitates — •Sascha B. Maisel[1], Won-Seok Ko[2], Jiali Zhang[3], Blazej Grabowski[1], and Jörg Neugebauer[1] — [1]Max-Planck Institut für Eisensforschung, Düsseldorf, Germany — [2]Ulsan University, Ulsan, Republic of Korea — [3]Massachusetts Insitute of Technology, Cambridge, USA

The properties of Ni-Ti nanoparticles differ from the properties of bulk Ni-Ti, yet they retain their characteristic shape memory effect. Austenitic Ni-Ti nanoprecipitates can be dispersed in metallic matrices and it has been speculated that this may lead to transformation-based strengthening due its intrinsic shape-memory property. Such an approach is considered promising to confer so-called “self-healing” features to alloys. Here, we present a combined experimental and theoretical study of such nanoprecipitates embedded coherently in Ti-V matrices. Using our knowledge of the Ni-Ti-V phase diagram based on a combination of density-functional theory and CALPHAD methods we were able to synthesize such alloys. Preliminary SEM investigations suggest nanoparticles of $\approx$ 200 nm can form in Ni-V matrices with $\approx$ 45 at. % V. Despite this progress, making samples large enough for mechanical testing remains a challenge. Thus, we study the properties of the compound using three-dimensional atomistic simulations based on the modified embedded atom method. We determine the conditions under which the martensitic transformation of such nanoparticles is triggered, which depends on the size of the particle, the composition of the surrounding matrix, temperature and strain state of the system.

MM 22.5 Mon 19:00 P4

Improved anodisation of aluminium thin films for flexible plasmonic applications — •Matthias Böhm[1], Fabian Patrovsky[1], Susan Derenko[1], Vera Fiehler[1], Stephan Barth[2], Hagen Bartzsch[2], Peter Frach[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik, TU Dresden, Deutschland — [2]Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik Dresden (FEP), Dresden, Deutschland

The future of optics heavily relies on reliably and easy-to-fabricate plasmonic materials that allow for the manufacturing of novel and versatile products and devices. Nanorod arrays (NRA), for instance, are fabricated by anodising aluminium thin films with acidic solutions [1]. However, large scale manufacturing of such structures so far has mostly shown not to be very reliable and reproducible [2].

We present an easy-to-use protocol [3] that firstly allows for the reliable substrate-bound anodisation of aluminium thin films and subsequent pore filling of anodised alumina matrices, while secondly easily promoting the NRA integration into mechanically flexible plasmonic devices. Replacing the template with an elastic material yields a novel, flexible and mechanically stretchable plasmonic composite, which allows for reproducible spectral tunability in the visible wavelength range [4].

[1] A. Eftekhari, ”Nanostructured Materials”, Wiley-VHC, (2008).
[2] M. Es-Souni and S. Habouti, Front. Mater. 1, 35706, (2014).
[3] F. Patrovsky et al., Thin Solid Films (2016) submitted.
[4] M. Böhm et al., Opt. Mater. Express (2016) submitted.

MM 22.6 Mon 19:00 P4

Theory of Polaron Band Narrowing and Phonon Renormalization due to Quadratic Electron-Phonon Coupling — •Pablo Garcia Risueno, Qiang Fu, and Claudia Draxl — Humboldt Universität zu Berlin, Physics Department and IRIS Adlershof

We present a novel theory of electron-lattice interaction beyond the linear-coupling regime. Based on the solution of a Holstein-Peierls-type model for quadratic electron-phonon coupling, we derive explicit analytical expressions for the eigenvalue spectrum of the Hamiltonian, resulting in a narrowing of bands as a function of temperature. Being nonperturbative, our formalism also applies in the strong-coupling case. It provides a starting point for potential applications to real materials by supplementing it with ab initio parameters.

MM 22.7 Mon 19:00 P4

Synthesis and functionalization of Li_2MnSiO_4 and $LiFe_{0.1}Mn_{0.9}PO_4$ for Li-ion batteries — •Kevin Häuser[1], Christoph Neef[1], Hans-Peter Mayer[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany — [2]Institut für Geowissenschaften, Universität Heidelberg, D-69120 Heidelberg, Germany

Two classes of materials are studied with respect to their applicability and optimisation for usage in Li-ion batteries. For hydrothermally synthesized $LiFe_{0.1}Mn_{0.9}PO_4$, the effect of the primary particle size and of hierarchical structuring of the nanosized active materials into micrometer-sized agglomerates by usage of organic additives and post-synthesis treatment is investigated. In contrast, Li_2MnSiO_4 was synthesized by an all-acetate precursor sol-gel process. Various carbon additives were tested to determine the optimal way of creating an embedding carbon nanomatrix to functionalize the materials. For both classes, the materials are characterised by SEM and XRD studies. The electrochemical properties are investigated by means of galvanostatic cycling and the influence of primary particle size and carbon structuring is discussed.

MM 22.8 Mon 19:00 P4

Complex Main-Group Halide Semiconductors Related to Perovskite: Aiding the Rational Design of Photovoltaics — •Anna J. Lehner[1], Douglas H. Fabini[2], Hayden A. Evans[2], Claire-Alice Hebert[2], Hengbin Wang[2,3], Michael L. Chabinyc[2], and Ram Seshadri[2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]MRL, UCSB, USA — [3]MC-CAM, UCSB, USA

Hybrid organic-inorganic lead halide perovskites have emerged as very promising materials for optoelectronic applications. It is interesting to ask whether related compounds, ideally containing less toxic heavy metals, can also show those remarkable properties.

Here we present our comprehensive approach of preparing, structurally and spectroscopically characterizing as well as computationally modeling the electronic structures of various lead-free complex metal halides using density functional theory methods.[1] We present bismuth halides and materials with optoelectronically active organic constituents and discuss distinguishing features for these functional materials, such as a defect-tolerant electronic structure and proximal lattice instabilities. By studying the correlations of composition, crystal structure and electronic structure of these compounds we focus on deepening the understanding of complex main-group metal halides' optoelectronic performance and provide a starting point for the design of new functional materials.

[1] Lehner, A.J., Fabini, D.H., Evans, H.A., Hébert, C.A., Smock, S.R., Hu, J., Wang, H., Zwanziger, J.W., Chabinyc, M.L., Seshadri, R. *Chem. Mater.* **27** (2015) 7137–7148.

MM 22.9 Mon 19:00 P4

Melting and solidification behavior of In nanoparticles embedded in crystalline Al and amorphous AlYFe — •Mark Stringe, Martin Peterlechner, Harald Rösner, Christian Simon, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

A reduction of the sample dimension to the nanoscale typically causes a reduction in thermal stability due to an increasing relevance of the surface contribution to Gibbs free energy. Free standing metallic nanoparticles show a melting point depression [1] whereas coherently embedded nanoparticles show an increase in transformation temperatures.

In the present work In nanoparticles are embedded in different matrices using the melt-spinning technique. The thermal behavior of these particles is analyzed using calorimetric measurements. Structural analysis is performed via transmission electron microscopy.

Focusing on the influence of interfaces between particle and matrix, nanoparticles are embedded in both an amorphous phase showing no coherent interfaces and a crystalline matrix showing (semi-)coherent interfaces. By systematic variation of cooling rates the amount of undercooling is deduced to obtain the activation energy for crystal nucleation. Nanoparticles embedded in the amorphous phase behave more like free standing nanoparticles showing a larger undercooling than nanoparticles embedded in a crystalline phase.

[1] Buffat P, Borel J-P. Phys Rev A 13, 2287 (1976)

MM 22.10 Mon 19:00 P4

Numerical studies of the nucleation kinetics associated with interfaces in fcc binary systems — •M. Ajmal Choudhary and Julia Kundin — Department of Engineering Sciences, Universität Bayreuth

The phase-field crystal (PFC) technique is a widely used approach for modeling crystal growth phenomena with atomistic resolution on mesoscopic time scales. We use a two-dimensional PFC model for a binary system based on the work of Elder et al. [Phys. Rev. B 75, 064107 (2007)] to study the effect of the curved, diffuse solid-liquid interface on the interfacial energy as well as the nucleation barrier. The calculation of the interfacial energy and the nucleation barrier certainly depends on the proper definition of the solid-liquid dividing surface and the corresponding nucleus size. We define the position of the sharp interface at which the interfacial energy is to be evaluated by using the concept of equimolar dividing surface (re) and the minimization of the interfacial energy (rs). The comparison of the results based on both radii shows that the difference re*rs is always positive and has a limit for large cluster sizes which is comparable to the Tolman length. Furthermore, we found the real nucleation barrier for small cluster sizes, which is defined as a function of the radius rs, and compared it with the classical nucleation theory. The simulation results also show that the extracted interfacial energy as function of both radii is independent of system size, and this dependence can be reasonably described by the nonclassical Tolman formula with a positive Tolman length.

MM 22.11 Mon 19:00 P4

DFT Modelling and Size Evolution of Precipitate Clusters — •Tobias Stegmüller and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

One of the key roles in the manufacturing of modern metal alloys is the understanding of precipitation processes taking place during thermal treatments and their influence on many material parameters like hardness or corrosion resistance. While a lot of these processes are qualitatively well understood their quantitative control is still covered by empirical approaches.

One approach for the theoretical modelling of precipitation is the so-called cluster dynamics, by which the temporal evolution of the size distribution of precipitates can be simulated. This model was applied successfully in literature for several times to the formation of a single phase with spherical precipitate shape.

Our aim is to extend the model to more complex systems. One first step is the adaption to non spherical precipitate shapes, which needs an energetic modelling of the configurational space of all possible shapes. To perform this task we use DFT based Monte Carlo simulations and incorporate the results into the cluster dynamics formalism.

In our contribution we will show the results of our approach for the formation of the well known plate shaped Guinier Preston zones in AlCu.

MM 22.12 Mon 19:00 P4

Transmission electron microscopic examination of the precipitation growth in aluminium 2195 — •Johannes Luderschmid, Christian Felber, and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

For aerospace applications the aluminium alloy 2195 is due to its alloying elements and microstructure one of the most interesting materials, as it shows a high strength and simultaneously a low density. Especially the formation of precipitates (T1 phase (Al2CuLi) and θ' phase (Al2Cu)) controls the strength of the material. The formation of precursors like solute enriched regions (Guinier-Preston Zones) at room temperature is a further ability of the aluminium alloy 2195. In this study the influence of different pre-treatment (natural aging, direct quenching) and different annealing conditions (time, temperature) after the solution annealing is studied with respect to the T1 and θ' precipitation growth. In particular the influence of natural aging is investigated, as here precursor phases are formed, which already reduce the chemical driving force for the further precipitation growth during the heat treatment. The kinetics of precipitate formation and growth were investigated using transmission electron microscopy and differential scanning calorimetry. The temperature and the time are the critical parameter for a diffusion process like the precipitate growth. For that reason these parameters were modified for the heat treatment in order to identify a difference in the growing of the precipitations.

MM 22.13 Mon 19:00 P4

Synthesis of nanostructured ZnO-based gas sensing devices — •Hanaa Seso, Stefan Ostendorp, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-University, Wilhelm-Klemm-Str.10, Münster, Germany

Solid state sensing devices for detecting gases and determining their composition gain increasing interest in recent years. Applications exist in many different fields as e.g. industrial emission analysis or vehicle emission control. In the present work, the well-known chemo-resistive effect of ZnO is used. Which is found in the presence of an oxidizing or reducing gas species. In combination with a 3d nano-structuring procedure based on anodic-aluminum-oxides, a large sensor surface is obtained to enhance the sensitivity compared to a flat 2d sensor structures. ZnO nano-tubes with different diameters and wall thicknesses were prepared by atomic layer deposition within the pores of porous anodic alumina membranes (PAAMs). Gold electrodes for electrical read-out were fabricated by physical vapor deposition. The morphology of the ZnO-based CO sensors were investigated by electron microscopy and atomic force microscopy, and functionality was characterized using a custom-build test station. Structural differences were tried to correlate to the sensing response of the sensor structure under different ambient temperatures and different CO concentrations. The results are analyzed systematically to draw conclusions on the underlying physical mechanisms.

MM 22.14 Mon 19:00 P4

Perfectly-Ordered Nanostructure Arrays as Potentially Promising Building Blocks for Constructing High-Performance Devices — •Huaping Zhao, Rui Xu, Max Sommerfeld, Liying Liang, Min Zhou, Yang Xu, and Yong Lei — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Nanostructure arrays of functional materials have drawn great current attentions for different device applications. Among the various techniques developed for fabricating arrayed nanostructures of functional materials, template-based nanostructuring technique with porous anodic alumina membrane as template becomes more and more attractive owing to the superior geometrical characteristics. Herein, we demonstrate the utilization of perfectly-ordered porous anodic alumina membrane as template for the preparation of perfectly-ordered nanostructure arrays of functional materials. By employing the perfectly-ordered porous anodic alumina membrane as template, the as-obtained nanostructure arrays have highly-controllable and perfectly-ordered structure features in large scale, which enable them to be of great advantage for the performance improvement of devices, especially for the energy conversion and energy storage devices, including solar water splitting cells, supercapacitors, and batteries, etc.

MM 22.15 Mon 19:00 P4

Measurement and Modelling of the Efficiency of ortho/para Catalysts for Hydrogen — •Sebastian Mirz, Florian Altenbrand, Robin Grössle, and Bennet Krasch — Tritium Laboratory Karlsruhe (TLK), Institute for Technical Physics (ITEP), Karlsruhe Institute of Technology (KIT)

The equilibrium ratio between ortho and para hydrogen is 3:1 at room temperature, whereas para hydrogen would be the only present species at absolute zero. The conversion between these two species is suppressed with time constants of the order of thousand hours in the gas phase and ten hours in the liquid phase, but can be catalytically accelerated. The TLK develops an analysis system for the hydrogen isotopologue concentration in the liquid phase in a cryogenic distillation collumn, based on IR absorption spectroscopy. An ortho/para catalyst is needed for the calibration of this system, due to the influence of the ortho/para ratio on the IR spectra. Therefore, an experiment is installed for the investigation of ortho/para catalyst performance at temperatures between 77 K and 400 K, to provide the necessary data for the design of this catalyst. The unique application of a Raman spectroscopy system enables the model-free real-time monitoring of the ortho/para ratio during conversion. This allows the extraction of the catalyst efficiency and additionally the distinction between physisorption and chemisorption processes. This contribution presents results of the measurement and modelling of the catalyst performance of an iron oxide catalyst.

MM 22.16 Mon 19:00 P4

Influence of metal oxides on sulfation kinetics of sodium chloride and chlorine induced corrosion — •Sebastian Pentz[1], Daniel Ott[1], Ferdinand Haider[1], and Ragnar Warnecke[2] — [1]Univ. Augsburg, Inst. f. Physik, 86135 Augsburg —

[2]Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion leads especially in waste-to-energy-plants to massive problems. At prevalent temperatures around 500°C-600°C corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlorides. This reaction requires an atmosphere containing SO_2, H_2O, O_2 and releases HCl/Cl_2. In this work the sulfation kinetics for different parameters, like temperature, gas stream, gas components or the influence of catalytic additives is examined. The conversion rate is strongly dependent on the transformation of SO_2 to SO_3, which is catalyzed by the presence of iron oxides like Fe_2O_3 or Fe_3O_4. Further experiments are done with Al_2O_3 which is supposed to be inert in the sulfation reaction or with CaO in order to examine whether a desulphurization process can be detected. In addition to the study of the reaction rate it is possible to characterize the metal loss of samples simultaneously. Furthermore the behaviour of chlorine during the process of the corrosion was investigated. Principles of the reaction conditions in waste-to-energy-plants, especially at the superheaters, are shown and laboratory experiments regarding the kinetics of sulfation reactions are presented.

MM 22.17 Mon 19:00 P4

Crystallization of coated nanoparticles — •Christine Walter[1], Christian Klein[1], Indranath Chakraborty[2], Wolfgang Parak[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-University, D- 60438 Frankfurt am Main, Germany — [2]Department of Physics, Philipps-University of Marburg, D-35037 Marburg, Germany

Nanoparticles and nanoparticle assemblies display a range of properties that can diverge from classical observed properties in the colloidal regime [1]. Gold Nanoparticles coated with ω-functionalized alkane thiols, also called nanoions, can be crystallized in a diamond-like lattice , if their functionalized layers carry opposite surface charges [2]. This novel type of metamaterial presents a well-ordered three-dimensional assembly of crystalline nanoparticles with lattice parameters of about 20 nm. However, so far no electrical or magnetic characterizations of these nanoparticle crystals have been performed.

In this contribution, we report on the technique of nanoparticle crystallization following the recipe given in [2] and we will discuss the influence of different parameters like temperature and solvent on the size of the nanoparticle crystals and discuss first magnetic measurements on these crystallized nanoparticles.

[1] B. A. Grzybowski, CrystEngComm 16, 9368 (2014). [2] A.M. Kalsin et al., Science 312, 420 (2006).

MM 22.18 Mon 19:00 P4

The new Lithography Scanner of BL1 at DELTA — •Jennifer Bolle[1], Michael Paulus[1], Christian Sternemann[1], Georg Jülicher[1], Thorsten Witt[1], Joachim Schulz[2], Thomas Beckenbach[2], Pascal Meyer[3], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU-Dortmund, D-44221 Dortmund, Germany — [2]microworks GmbH, Schnetzlerstr 9, 76137 Karlsruhe, Germany — [3]Karlsruhe Institute of Technology, Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

There is a great demand for increasingly smaller micromechanical components. Deep X-ray lithography is a process to produce high quality microstructures with a lateral resolution in the μm-range, high aspect ratio and low sidewall roughness [1,2]. The structures are transferred by a shadow projection to a photosensitive resist [3]. At beamline 1 of DELTA synchtrotron source a new X-ray lithography scanner (Jenoptik scanner (DEX01)) provided by BESSY was implemented and commissioned. The setup was characterized using test structures, exploiting different filters, bottom doses, and thermal conditions. This way optimized exposure parameters were determined and finally structures of industrial quality standards were produced. [1] A. Risse, /Fertigungsverfahren der Mechatronik, Feinwerk-und Präzisionsgerätetechnik/, Springer, 503 (2012); [2] A. del Campo, C. Greiner, /Journal of Micromechanics and Microengineering /17(6), R81 (2007); [3] G. Feiertag et al., /Applied Physics Letters /71(11), 1441 (1997).

MM 22.19 Mon 19:00 P4

Morphology of lithium-ion containing block copolymer electrolytes for rechargeable lithium-ion batteries — •Yinong Zhang, Ezzeldin Metwalli, Bernhard Springer, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Block copolymers (BC) electrolytes have been recently investigated as solid-state membranes for lithium-ion batteries. Nanostructured BC electrolyte contains both, the ionic conducting as well as the high-tensile polymer domains, enabling both, high ionic conductivity and improved mechanical stability. Since the diffusion path of the lithium-ions only follows the percolation path of the ionic conducting domain, the morphology of the BC electrolyte is an essential parameter. Theoretical studies have recently reported that the BC electrolyte phase diagrams significantly deviate from the conventional BC phase diagrams due to electrostatic interactions between polar chains and the alkali metal-ions. The morphology of ion-containing BC electrolyte was investigated using SEM and SAXS. In the current study, morphological deviation compared with that of the conventional BC phase diagrams in consistent with the theoretical studies is experimentally proved. Conductivity measurements of the Li-salt containing BC hybrid films were examined for different morphologies using impedance spectroscopy.

MM 22.20 Mon 19:00 P4

Multiplexed sensing of small molecules with silicon nanowire field effect transistors — •Stephanie Klinghammer[1], Tetiana Voitsekhivska[2], Clemens Kirschbaum[3], Larysa Baraban[1], and Gianaurelio Cuniberti[1,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Institute of Electronic Packaging Technology, TU Dresden, 01062 Dresden, Germany — [3]Department of Psychology, TU Dresden, 01062 Dresden, Germany — [4]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

The simultaneous detection of multiple targets within a single chip on a point-of-care device is attracting great attention within bio- and nanotechnology areas for more than decade[1]. Here, we demonstrate a multiplexed, label-free and real-time detection platform for small molecules like hormones, steroids, and viruses based on silicon nanowire field effect transistors (SiNW FETs). SiNW FETs are connected to a CMOS chip enabling the simultaneous readout of up to 32 FETs [2]. We particularly focus on the sensitive and selective binding of the target cortisol by using aptamers as receptors - allowing high sensitive screenings in more physiological conditions[3]. Finally we show the working principle in form of the biochipboxwhich serves as a portable, electro-microfluidic device facilitating the versatile and reliable detection of multiple samples on only one single sensor device. (1) Patolsky, F. et al., Nanomed. 2006, 1 (1), 51-65.; (2) Voitsekhivska, T. et al., IEEE, 2014; pp 173-178.; (3) Römhildt, L. et al., ACS Appl. Mater. Interfaces 2013, 5 (22), 12029-12035.

MM 22.21 Mon 19:00 P4

Equilibrium shapes of large nanoparticles: Wulff-construction on the atomic scale — •Magnus Rahm and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Finding the equilibrium shape of nanoparticles is a great challenge. While the classical Wulff construction provides a solution given a set of pre-defined surface energies in the continuum limit, the predictions are unreliable for medium sized nanoparticles when edge and corner sites have a sizeable effect the total energy. On the other end, numerous efforts have been made to find the global minimum shape without restrictions to crystal lattices, yet the complexity of the resulting optimization problem limits predictions to nanoparticle sizes of a few hundred atoms or less. Here, we explore the middle ground between large nanoparticles, which can be captured using the Wulff construction and very small nanoclusters. To this end, a computational technique based on Monte Carlo sampling in the variance-constrained semigrand canonical ensemble has been developed. We apply the method to a number of transition metals and demonstrate the flatting of the energy landscape with increasing particle size and describe its transition to the Wulff construction in the continuum limit. The method is also applied to particles with icosahedral symmetry, which are shown to have a much more rugged energy landscape and thus are more likely to exhibit a discontinuous size distribution.

MM 22.22 Mon 19:00 P4

Abnormal coarsening of nanoscale microstructures goes fractal — •Christian Braun[1], Jules M. Dake[2], Carl Krill[2], and Rainer Birringer[1] — [1]Experimental Physics, Universität des Saarlandes, Germany — [2]Institute of Micro and Nanomaterials, Universität Ulm, Germany

Despite the supposed rarity implicit in its name, abnormal grain growth (AGG) appears to be a rather common mode of coarsening in nanocrystalline materials, regardless of composition or synthesis route. In inert-gas-condensed nanocrystalline Pd90Au10, thermally induced coarsening fulfills the criteria for AGG, but with an unusual twist: here, the subpopulation of abnormally growing grains sends offshoots in many directions into the surrounding matrix, much like a tumor spreading into nearby tissue! The resulting irregular growth fronts manifest a fractal-like morphology instead of the smooth interfaces observed in conventional samples. We have captured this phenomenon using orientation imaging based on electron backscatter diffraction and obtained a fractal dimension of about 1.2 for the grain perimeter, which is reminiscent of percolation processes, the migration of domain walls in a random field of pinning centers or fractal lines on ranked surfaces.

MM 22.23 Mon 19:00 P4

ArF-excimer laser irradiation of gold coated float glass - formation and implantation of gold nanoparticles — •Maximilian Heinz[1], Manfred Dubiel[1], Leon Avakyan[2], Aram Bugaev[2], Lusegen Bugaev[2], Jürgen Ihlemann[3], and Jörg Meinertz[3] — [1]Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle (Saale), Germany — [2]Southern Federal University, Zorge Str. 5, 344090 Rostov-on-Don, Russia — [3]Laser-Laboratorium Göttingen e.V., Hans-Adolf-Krebs-Weg 1, D-37077 Göttingen, Germany

In this study, plasmonic Au nanostructures in soda-lime-silicate float glasses have been generated by gold coating and ArF-excimer laser irradiation (193 nm) of the glass surface. The formation of Au nanoparticles could be verified by the surface plasmon resonances between 530 and 600 nm, which were obtained by optical spectroscopy. Furthermore, the implantation of these nanoparticles into the glass as a consequence of melting of the glass surface by the laser has been investigated by means of electron microscopy (SEM and TEM). Here the absorption of the glass at the laser wavelength plays an important role. The implantation of the nanoparticles into the glass is an important condition to generate corrosion resistant laser marks, for example micro patterns, which are of specific interest for applications of nanoplasmonics, nanoantennas and labeling by holograms.

MM 22.24 Mon 19:00 P4

Planarization and pattern transfer at ultra-smooth aluminium surfaces — •Jens Bauer, Frank Frost, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Metal mirrors are of increasing interest for the technological progress in EUV/XUV lithography, x-ray and synchrotron optics. Recently, we have presented a direct surface figuring technology, which is based on reactive ion beam etch (RIBE) processing. The use of sub-aperture ion beams allows the deterministic machining of optical Al surfaces while preserving the surface roughness almost in its initial state. Now we apply this promising technique for an advanced customization of the Al surface topography. Two cases are distinguished: 1) Surface planarization experiments are performed applying a sacrificial resist layer. Typically, several hundred nanometres of resist allow for a geometrical levelling of disturbances within the surface micro-roughness and waviness. This smooth resist topography is then transferred into the Al surface. RIBE process optimization is performed by variation of the gas composition and ion beam machining geometry to achieve a resist/Al selectivity in the order of unity. 2) Al surfaces are structured by topography transfer of a patterned resist layer via RIBE. The proportional pattern transfer is controlled by the resist/Al selectivity. The engraving of regular ultra-shallow grid patterns into aluminium is performed by a damped proportional transfer. The processes are evaluated by AFM and WLI topography measurements. A PSD analysis allows for the quantitative assessment of topography features.

MM 22.25 Mon 19:00 P4

Modeling the electrocaloric effect in ferroelectric solid solutions — •Anna Grünebohm[1], Takeshi Nishimatsu[2], and Ralf Meyer[3] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institute for Materials Research, Tohoku University, Japan — [3]Department of Mathematics and Computer Science, Laurentian University, Sudbury, Canada

The electrocaloric effect (ECE) is the adiabatic temperature change of a material in a varying external electrical field. The ECE is promising for novel cooling devices [1]. However, in many ferroelectrics the large ECE is restricted to a narrow temperature interval. Solid solutions such as $\mathrm{Ba}_x\mathrm{Sr}_{1-x}\mathrm{TiO}_3$ are promising to tune the operation range. We discuss possible routes of modeling disordered solid solutions by means of *ab initio* based molecular dynamics simulations [2,3]. Furthermore, we present direct simulations of the ECE for $\mathrm{Ba}_x\mathrm{Sr}_{1-x}\mathrm{TiO}_3$ [4].

[1] X. Moya, *et al.*, Nature Mater. **13**, 439 (2014).
[2] T. Nishimatsu *et al.*, J. Phys. Soc. Japn. **85**, 114714 (2016).
[3] S. Tinte *et al.*, J. Phys.: Condens. Matt. **16**, 3495 (2004).
[4] M. Marathe, *et al.*, Phys. Rev. B **93**, 054110 (2016).

MM 22.26 Mon 19:00 P4

Tuning of the optical properties from alloy nanoparticles with varied compositions sputtered from one target — •Wiebke Reichstein[1], Alexander Vahl[1], Julian Strobel[2], Olexandr Polonskyi[1], Thomas Strunskus[1], Lorenz Kienle[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Synthesis and Real Structure, Kaiserstr. 2, 24143, Kiel, Germany

Optical properties like particle plasmon polaritons of elemental noble metal nanoparticles were well studied over the past years. Recently, alloy metal nanoparticles have generated increasing interest due to their additional functionalities. In this work the optical properties of multiple stacks of silver-gold alloy nanoparticles in a transparent matrix are investigated. Nanoparticles were deposited using a Haberland type single DC magnetron gas-aggregation-source and are incorporated into a silicondioxide matrix (pulsed reactive DC magnetron sputtering). UV-vis transmission spectra were obtained on samples where the gold concentration in the nanoparticles was varied from 60 to 75 at% leading to corresponding shifts of the plasmon resonance peak positions. Furthermore, the influence of nanoparticle agglomeration on the appearance of the plasmon absorption band was analyzed which could allow optical control of the deposition process.

MM 22.27 Mon 19:00 P4

Nano Structuring with New High-Resolution and Longtime-Stable Liquid Metal Ion (Alloy) Sources — •Torsten Schneider-Rahder[1,2], Achim Nadzeyka[2], Lars Bruchhaus[2], Sven Bauerdick[2], Paul Mazarov[2], Michael Kahl[2], and Andreas-Dirk Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Raith GmbH, Dortmund

To generate structures on scales of micro- or nanometers, metal ions and clusters can be used, because their de Broglie wavelength is much smaller than that of light. This allows a higher resolution also of structures smaller than the wavelength of light. In fact, the resolution limit is more on the side of the instrumentation than due to the de Broglie wavelength, being of the order of only $\lambda = h/\sqrt{2mE} = 20$ fm (mass 70 amu, E = 30 keV). Metal ions emitted by liquid metal ion sources (LMIS) are bundled to a focused ion beam (FIB). Most of the commercial applications use Ga^+ ions; here drawbacks exist due to unwanted implantation. Thus the fundamental goal of the current project is to investigate alloys consisting of different other metals, which show a eutectic behavior and are suitable to achieve a longtime-stable operation of the LM(A)IS. First, the sputtering yield of a LMAIS emitting Au^+, Au^{++} and Si^{++} ions will be analyzed according to the beam current and the dwell time. For these measurements, samples of Si, Cr, Au and others will be used. Subsequently, more parameters will be varied in order to maximize the removal rate and the resolution. Similar investigations will be conducted using other alloys containing different metals (basically Bi) to optimize their operating conditions as well.

MM 22.28 Mon 19:00 P4

Ferrite filled carbon nanotubes vs. ferrite nanoparticles as anode materials for lithium ion batteries — •Lucas Möller[1], Alexander Ottmann[1], Rüdiger Klingeler[1,2], Rasha Ghunaim[3], and Silke Hampel[3] — [1]Kirchhoff Institute of Physics, Heidelberg University — [2]Centre for Advanced Materials, Heidelberg University — [3]Leibniz Institute for Solid State and Materials Research (IFW) Dresden

Various nanosized ferrite $\mathrm{MFe_2O_4}$ (M = Fe, Co, Ni) materials incorporated into multiwalled carbon nanotubes (CNT) have been studied as anode materials for Li-ion batteries. Electrochemical measurements by means of cyclic voltammetry (CV) and galvanostatic cycling with potential limitation (GCPL) were carried out in Swagelok-type two-electrode cells against $\mathrm{Li/Li^+}$. In order to evaluate the benefits of the CNT shells, the results are compared to pristine ferrite $\mathrm{MFe_2O_4}$ nanoparticles. The CVs show typical redox activity associated with the conversion reaction $MFe_2O_4 + 8Li^+ + 8e^- \leftrightarrow M + 2Fe + 4Li_2O$. For the functionalised nanotubes, the data show in addition signatures of Li de-/intercalation into the CNTs. GCPL measurements reveal better cycling stability of the CNT-incorporated compared to the pristine ferrite nanoparticles.

MM 22.29 Mon 19:00 P4

Characterization of different *para*-quinones as electrode materials in Li-ion batteries — •Christina Schmidt[1], Yuquan Wu[1], Sebastian Hahn[2], Felix Hinkel[2], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Centre for Advanced Materials, Heidelberg University, Germany

The applicability of various *para*-quinones as electrode materials in lithium-ion batteries has been studied by means of cyclic voltammetry and galvanostatic cycling. The aza-*para*-quinones under study have been synthesized by classic condensation reactions with established procedures. Particular emphasis is given to the preparation of the solid electrodes and to the influence of the electrolyte. Our data imply that up to 3 Li^+-ions per molecule can be stored electrochemically, which, in the example of 5,7,12,14-tetraaza-6,13-pentacenequinone (TAPQ), are associated with reversible redox reactions at potentials between 1.8 and 3.0 V vs. Li/Li^+. Except for the first few cycles which show relatively high capacities above 300 mAh/g, the electrodes suffer from strong fading effects. No significant improvement of the cycling stability is observed when using different carbon additives or an ether-based electrolyte.

MM 22.30 Mon 19:00 P4

Grain boundary and triple junction segregation: Comparison between atom probe experiments and atomistic simulations — Rüya Duran, Daniel Beinke, •Sebastian Eich, and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

In nanocrystalline materials, the volume fractions of grain boundaries (GBs) and triple junctions (TJs) gain significance, justifying these defects as a major research topic. Excess solute segregation at those defects generally reduces the free energy of the system and may inhibit grain growth and lead to stabilization of nanocrystalline materials.

Atom probe tomography (APT) is a state-of-the-art technique with nanometer accuracy in order to obtain 3D information of the spatial chemical distribution, allowing conclusions about GB segregation amplitude and GB compositional width.

However, both the field evaporation process in APT experiments and the reconstruction algorithm *eo ipso* imply artifacts in the reconstructed sample, e.g. drastic differences of atomic densities in the GBs as compared to the bulk.

By comparing experimentally investigated two-component nanosized samples with realistic computer-simulated tricrystals, subjected to subsequent simulated evaporation, we reveal influences of the actual evaporation process on the reconstructed tip. Density fluctuations can directly be linked to different evaporation fields, which result from structural effects (e.g. different bonding in GBs) and/or different chemical species.

MM 22.31 Mon 19:00 P4

Viscoelastic and structural relaxation processes in Bombyx mori silk fibers studied by in situ X-ray scattering experiments — •Jan Rosigkeit[1], Igor Krasnov[1], and Martin Müller[2,1] — [1]Institut für experimentelle und angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Institut für Werkstoffforschung, Helmholtz-Zentrum Geesthacht

The mechanical properties of silk fibers are studied using an in situ combination of tensile tests with X-ray scattering experiments. We report our results about the vicoelastic relaxation. Structural relaxations in silk fibers exposed to tensile stress have been observed to take place on a very wide range of time scales from a few milliseconds to several hours. The phenomena can be well described by models based on fractional calculus. The time-dependence of the measured tensile force following a quasi-instantaneously applied external strain on the fibers can be understood in terms of a fractional viscoelastic relaxation function introducing memory effects by which the mechanical state of a fiber depends on its tensile history. The relaxation behavior could be well described with the fractional viscoelastic theory.

MM 22.32 Mon 19:00 P4

Optical characterization of thin-film electrode materials during electrochemical measurements — •Tim Theil, Nelly Sanchez, Yug Joshi, Susann Nowak, and Guido Schmitz — Institut für Materiawissenschaft, Universität Stuttgart

Thin-film battery electrodes are mainly characterized using electrochemical methods like cyclic voltammetry and chronopotentiometry. Using optical measurements additional insights into processes happening in the electrode materials or at the interfaces during cycling can be gained. Monitoring in-situ during lithiation and delithiation can give insight into chemical reactions or thickness changes. The approach is proven using lithium cobalt oxide (LCO) as an example for a cathode and lithium titanate (LTO) as an example for an anode. Both materials were prepared by ion beam sputter deposition on platinum coated silicon wafer with oxygen as reactive gas. LCO was crystallized by post annealing at 600°C whereas LTO was in situ annealed at 600°C. For the measurement a liquid cell with a three electrode setup was used where the used electrolyte was 1 molar LiClO4 in EC:DMC, the counter and the reference electrode was pure lithium metal. During cycling the sample was illuminated in a 45° angle by a tungsten source and each second a reflectance spectrum was acquired at 90° to the incoming beam. The reversible dependence of the optical properties on the charge state of the materials can be clearly shown.

MM 22.33 Mon 19:00 P4

Electrochemical Strain Microscopy for mapping ionic conductivity with high spatial resolution — •Nino Schön[1,2], Svenja Benning[1,2], Roland Schierholz[1], and Florian Hausen[1,2] — [1]Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, 52425 Jülich, Germany — [2]RWTH Aachen University, Institute of Physical Chemistry, 52074 Aachen, Germany

Devices for energy storage play an important role in our daily life but also in tackling fundamental problems towards a sustainable energy landscape. Currently challenging is the ability to store surplus energy and release it on demand. All-solid-state Lithium-Ion-Batteries (ASSLiB) present an attractive solution with high potential for further development. To realize improved solid state batteries, it is of utmost importance to understand the electrochemical and charge transport properties of promising energy materials at a relevant scale, especially the correlation between microstructure and local Li-Ion conductivity.

Within this contribution we introduce Electrochemical Strain Microscopy (ESM) as a method to investigate ionic conductivities with very high spatial resolution. ESM is based on Atomic Force Microscopy, a powerful tool to get insights into the surface characteristics at the nanometer scale. The Underlying principle of ESM is the link between the Li-Ion concentration and the molar volume. Ionic conductivity can be detected indirectly by applying a localized voltage pulse and inducing Li-Ion movement the resulting material strain can be quantified with subnanometer resolution. Hence, ESM allows for direct correlations between ionic conductivity and microstructure.

MM 22.34 Mon 19:00 P4

A detailed atomic investigation of the clustering and precipitation on a Friction-Stir-Welding simulated Al-Cu-Li(-Mg) alloy (AA2198) — •Danny Petschke, Frank Lotter, and Torsten Staab — Lehrstuhl für Chemische Technologie der Materialsynthese, Röntgenring 11, 97070 Würzburg

Al-Cu-Li-(Mg) alloys find wide applications in aviation and aerospace technology due to the reduction of weight and their high strength at the same time. After rolling sheets of these alloys, a defined heat treatment, following the solution annealing, leads to the formation of mainly T1-precipitates (Al2CuLi). These precipitates are highly efficient in blocking dislocation movements and, therefore, are responsible for the high strength of the alloy. When these sheets are joined by Friction-Stir-Welding (FSW), temperatures occurring in the Weld-Nugget (WN) are close to the material's solution treatment temperature (490-510°C). Hence, the T1-precipitates are completely dissolved in this region, which results in a significant hardness-drop of 25%. Obviously, only GP-zones/GPB-zones and CuMg-clusters of several Ångström in size are formed directly after welding by diffusion processes not understood in detail, yet. We followed the precipitation kinetics directly after Friction-Stir-Welding with DSC, SAXS and Positron-Annihilation-Spectroscopy (PAS). Therefore, a Welding-Simulator was developed to reproduce the temperature profile in the welded material.

MM 22.35 Mon 19:00 P4

Characterization of materials for all-solid-state batteries prepared by ion-beam sputtering — •Susann Nowak[1], Fabian Wunde[2], Juliane Mürter[1], Giulio Calcagno[1], Prianyka

Sharma[1], Yug Joshi[1], Tim Theil[1], and Guido Schmitz[1] — [1]Heisenbergstr. 3, 70563 Stuttgart — [2]Wilhelm-Klemm-Str. 10, 48149 Münster

All-solid-state batteries are discussed as a solution for the challenges lithium-ion batteries are facing in the moment. An all-solid-state battery is a complex system consisting of a cathode, an electrolyte, an anode and different current collectors. For the purpose of creating an all solid-state battery different materials for all of these components have to prepared and characterized. This contribution presents the properties of different battery materials which were successfully produced using ion-beam sputtering. In particular, the fabrication and properties of LFP, LMO, LCO, Sn, Si and LiPON as thin films are shown. All-solid-state batteries which were prepared using these materials are shown and were characterized by temperature dependent cyclic voltammetry and TEM investigations. It is shown that the cycling stability is largely dependent on the chosen anode material, when lithium and tin are compared.

MM 22.36 Mon 19:00 P4

Understanding chemical ordering in intermetallic clathrates — •Mattias Ångqvist and Paul Erhart — Department of Physics, Chalmers University of Technology, Sweden

Clathrates are periodic structures that provide a framework that can trap large, loosely bound species. Intermetallic clathrates often have low thermal lattice conductivity and high electric conductivity, which makes them interesting candidates for thermoelectric applications. These materials exhibit a great variability with respect to elemental composition and the distribution of the species, which provides flexibility for tuning properties but also poses a challenge with regard to developing a comprehensive understanding of these systems. Here, we demonstrate a method that can both accurately and efficiently sample this compositional space. We use density functional theory calculations to parametrize alloy cluster expansions (CE) to obtain *ab-initio* accuracy in Monte Carlo simulations that can exhaustively sample the compositional space. We apply this methodology to study the chemical ordering and related effects in the binary clathrates $Ba_8Al_xSi_{46-x}$, $Ba_8Al_xGe_{46-x}$, $Ba_8Ga_xGe_{46-x}$, and $Ba_8Ga_xSi_{46-x}$ in terms of composition and temperature. We validate our method by predicting the site occupancy factors (SOFs) and achieve excellent agreement with experimental results. This validation enables us to provide a rationale for the extreme SOF behavior with varying Al content by looking at the actual interactions found in the CE. Finally, we address the contributions of chemical ordering on heat capacity and lattice expansion.

MM 22.37 Mon 19:00 P4

In situ functionalization and spectroelectrochemical characterization of gallium nitride surfaces for novel hybrid sensing platforms — •Princia Salvatore, Eugen Speiser, and Norbert Esser — Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Schwarzschildstr. 8, 12489 Berlin

Inspired by the existing semiconductor technology and encouraged by the unique set of optical and electronic properties of gallium nitride (GaN), the integration of such a material in novel sensing platforms has been attempted proceeding through a solution-based in situ modification of GaN surfaces via a phosphonic acid (PA) linkage. In contrast to other harsher functionalization routes, this approach offers the opportunity to prepare samples in solution with no need of removing oxide layers, and to exploit the side/end groups of PA derivatives for GaN surfaces terminating with different chemistries. PA adsorbates based on terpyridine are under investigation with the aim of exploring robust surface-confined layers for metal ions chelation and sensing in solution. A dual investigation by interfacial electrochemistry and optical spectroscopy (Raman and photoluminescence analysis), referred to as spectroelectrochemistry, serves to verify efficiency of the surface modification scheme and sensitivity of the sensing route, which applies to functionalized GaN crystals as planar or nanostructured surfaces. Under a monochromatic light excitation and bias, insight into interfacial processes (surface assembly, charge transfer, band bending, etc.) is gained towards the creation of novel hybrid sensors, based here on the highly controlled deposition of PA derivatives on GaN electrodes.

MM 22.38 Mon 19:00 P4

Investigation of molecular orientation in individual metal-organic nanowire by polarized raman spectroscopy and simulation — •Yanlong Xing[1], Eugen Speiser[1], Dheeraj Kumar Singh[2], Petra Dittrich[3], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften, ISAS e.V., 12489 Berlin, Germany — [2]Department of Chemical Physics, Jacobs University, 28759 Bremen, Germany — [3]Department of Biosystems Science and Engineering, ETH Zürich, 8093 Zürich, Switzerland

To study the molecular self-organization in conductive metal-organic nanowire, single gold-tetrathiafulvalene (Au-TTF)nanowires were analysed using non-destructive polarized Raman spectroscopy at room temperature. A first investigation was done for neutral tetrathiafulvalene (TTF) crystal. Based on the density functional theory calculation of molecular Raman tensor and simulation of depolarization ratio, the orient of TTF molecules in a single TTF crystal was revealed. The high correlation between the results from this work and that of reported work proved the efficiency of the proposed method in this work. Afterwards, both the experimental and simulation method for TTF crystal was applied to study a single Au-TTF nanowire. It was indicated that there were at least two different molecule configurations in the wire, both tilted with respected to the long axis of the wire. The 3D model of sing Au-TTF wire showed a vivid image of molecular configurations in the wire. Compared to the proposed mechanism in reported work, this improved model can better explain the growth mechanism of Au-TTF wires with various morphologies.

MM 22.39 Mon 19:00 P4

Mechanical alloying of Ti-25Ta for biomedical applications: Effect of milling parameters — •yanfei Sui[1], Mariana Calin[1], Sergio Scudino[1], Chunming Zou[2], Zunjie Wei[2], and Jürgen Eckert[3] — [1]IFW Dresden, Institute for Complex Materials, 01171 Dresden, Germany — [2]National Key Laboratory for Precision Heat Processing of Metal, Harbin Institute of Technology, Harbin 150001, China — [3]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

The influence of milling parameters, such as milling time (10h-80h), milling speed (200rpm, 250rpm, 300rpm), as well as the initial powder morphology, have been investigated. The microstructure of the milled powder has been characterized by scanning electron microscopy, coupled with X-ray diffraction. The results indicate that, the interval milling mode that carried out with a speed of 250rpm, shows optimized mechanical alloying effect. At the initial stages of ball milling a significant broadening of the diffraction peaks was observed, which can be linked to phason strain of the quasilattice. With increasing milling time, the diffraction signals belonging to β phase were no longer observed, indicating a complete transformation of β phase to α phase. The milled powder can be further used to synthesize compacts with a low elastic modulus for biomedical applications.

MM 22.40 Mon 19:00 P4

Mechanical alloying of Ti-25Ta for biomedical applications: Effect of milling parameters — •yanfei Sui[1], Sergio Scudino[1], Chunming Zou[2], Zunjie Wei[2], Mariana Calin[1], and Jürgen Eckert[3] — [1]IFW Dresden, Institute for Complex Materials, 01171 Dresden, Germany — [2]National Key Laboratory for Precision Heat Processing of Metal, Harbin Institute of Technology, Harbin 150001, China — [3]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

The influence of milling parameters, such as milling time (10h-80h), milling speed (200rpm, 250rpm, 300rpm), as well as the initial powder morphology, have been investigated. The microstructure of the milled powder has been characterized by scanning electron microscopy, coupled with X-ray diffraction. The results indicate that, the interval milling mode that carried out with a speed of 250rpm, shows optimized mechanical alloying effect. At the initial stages of ball milling a significant broadening of the diffraction peaks was observed, which can be linked to phason strain of the quasilattice. With increasing milling time, the diffraction signals belonging to β phase were no longer observed, indicating a complete transformation of β phase to α phase. The milled powder can be further used to synthesize compacts with a low elastic modulus for biomedical applications.

MM 22.41 Mon 19:00 P4

An Improved Method for Point Deflection Measurements on Rectangular Membranes — •Benoit Merle[1], Kyle Nicholson[1], Erik Herbert[2], and Mathias Göken[1] — [1]Materials Science & Engineering 1, Friedrich-Alexander-University Erlangen-Nürnberg (FAU) — [2]Department of Materials Science & Engineering, Michigan Technological University

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

MM 23: Invited talk Srolovitz

Time: Tuesday 9:30–10:00 Location: BAR 205

Invited Talk MM 23.1 Tue 9:30 BAR 205
Integration of Grain Boundary Mechanics and Migration — •David Srolovitz, Jian Han, Spencer Thomas, and Vaclav Vitek — University of Pennsylvania, Philadelphia, PA USA

Most grain boundary (GB) properties are modeled as if they were associated with isolated phenomena; these include GB mobility, GB sliding, GB interactions with lattice dislocations, GB roughening, GB shear coupling,... The result of these efforts has largely been phenomenological models with little quantitative predictability. In this presentation, I will outline an approach that has its foundations in grain boundary bicystallography which, when coupled with, some simple statistical mechanics ideas, show how these phenomena are intimately coupled. The presentation will outline the underlying theoretical ideas and demonstrate these with molecular dynamics and Monte Carlo simulations.

MM 24: Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs

Time: Tuesday 9:30–12:15 Location: HSZ 02

Invited Talk MM 24.1 Tue 9:30 HSZ 02
New twists in biological photonics: circular polarisation and beyond. — •Pete Vukusic, Luke McDonald, and Ewan Finlayson — University of Exeter, Exeter, UK.

The evolution of structural colour mechanisms in many biological systems has given rise to many specialised and often highly functional optical effects both in animals and in plants. Recent scientific works yielded several examples that are being developed for use across technology. Among many thousands of biological systems, a distinctive example involving circular polarisation (CP) was described by Michelson himself: the scarab beetle Chrysina resplendens. Its exoskeleton has a bright, golden appearance that reflects both right-handed and left-handed CP light. The chiral nanostructure responsible for this is a helicoid comprising twisted birefringent dielectric planes. This presentation revisits the C. resplendens beetle, correlating details of its CP reflectance spectra directly with detailed analysis of its morphology that includes a chiral multilayer configuration comprising two chirped, left-handed, helicoids separated by a birefringent retarder. The system's optical behaviour is modelled using a scattering matrix simulation, where the optical roles of each component of the morphological substructure are elucidated. The C. resplendens' model is presented here, alongside summaries of other inspirational biological structural colour generation strategies, as a key example of highly adapted optical design.

Invited Talk MM 24.2 Tue 10:00 HSZ 02
Bio-inspired materials and structures for technology and architecture — •Thomas Speck — Plant Biomechanics Group & Botanic Garden, University of Freiburg

Biological structures and materials are typically multi-layered, hierarchically structured, finely tuned and highly differentiated based on the combination of a few basic molecular components. This leads to materials and structures that are characterized by multiple networked functions and (often) possess excellent mechanical properties, a pronounced adaptability to changing environmental conditions and manyfold self-x-properties.

During the last decades biomimetics, i.e. using living organisms as inspiration for technical developments products, has attracted increasing attention as well from basic and applied research as from various fields of industry. Biomimetics has a high innovation potential and offers the possibility for the development of sustainable technical products and production chains. On the one hand, novel sophisticated methods for quantitatively analyzing and simulating the form-structure-function-relationship on various hierarchical levels allow new fascination insights in multi-scale mechanics and other functions of biological structures, materials and surfaces. On the other hand, recent developments in computational design and simulation together with new production methods enable for the first time the transfer of many outstanding properties of the biological role models into innovative biomimetic products for reasonable costs which makes them interesting for applications in many fields of technology and building construction.

Invited Talk MM 24.3 Tue 10:30 HSZ 02
Cellulose bio-inspired hierarchical structures — •Silvia Vignolini — Lensfield Road Cambridge CB2 1EW UK

Nature's most vivid colours rely on the ability to produce complex and hierarchical photonic structures with lattice constants on the order of the wavelength of visible radiation. A recurring strategy design that is found both in the animal and plant kingdoms for producing such effects is the helicoidal multilayers. In such structures, a series of individual nano-fibers (made of natural polymers as cellulose and chitin) are arranged parallel to each other in stacked planes. When distance between such planes is comparable to the wavelength of light, a strong polarised, colour selective response can be obtained. These helicoidal multilayers are generally structured on the micro-scale and macroscopic scale giving rise to complex hierarchical structures.

Biomimetic with cellulose-based architectures enables us to fabricate novel photonic structures using low cost materials in ambient conditions. Importantly, it also allows us to understand the biological processes at work during the growth of these structures in plants. In this talk the route for the fabrication of complex bio-mimetic cellulose-based photonic structures will be presented and the optical properties of artificial structures will be analyzed and compared with the natural ones.

15 min break

Invited Talk MM 24.4 Tue 11:15 HSZ 02
Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing — •Vladimir Tsukruk — School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, USA

I discuss recent results from our research group on designing flexible and strong responsive polymer and biopolymer nanocomposite materials and structures for advanced flexible sensing and electronic applications. Ultrathin silk fibroin proteins and chemically modified cellulose nanocrystals were assembled in order to control intimate assembly with graphene oxide sheets with controlled surface chemical composition on planar and curved substrates. We demonstrated flexible laminated bionanocomposites with developed biointerphases that facilitate extremely high elastic modulus, bending flexibility, and toughness. Both experimental and computational methods were undertaken to address silk fibroin adsorption at heterogeneous surfaces of graphene oxide with different degrees of oxidation. Graphene oxide and reduced graphene oxide sheets at various levels of oxidation were compared with silicon dioxide (SiO2) as a benchmark substrate. We concluded that silk fibroin readily forms single molecule proto-nanofibrils with β-sheet structures on oxidized graphene oxide surfaces but aggregated globular structures on the hydrophobic surfaces. Finally, electrochemical-assisted photolithography has been utilized for high spatial resolution conductive patterning of these nanocomposites with high local electrical conductivity, sharp boundaries, and optical transparency. Some peculiar features of these flexible bionanocomposites can be explored for tactile recognition, remote sensing, and low-noise SERS substrates.

Invited Talk MM 24.5 Tue 11:45 HSZ 02

3D laser nano-printing of rationally designed materials — •Martin Wegener — Karlsruhe Institute of Technology, Karlsruhe, Germany

Broadly speaking, 3D structures and materials can be designed by using the human brain, computer-based (topology) optimization, or inspiration from nature. Regardless of how a 3D blueprint has been obtained, it eventually needs to be manufactured. 3D laser printing on the micro- and nanometer scale has become a versatile and reliable workhorse for accomplishing this task. Here, we review recent examples from our group. This includes micropolar metamaterials with behavior beyond ordinary continuum mechanics, metamaterials with effectively negative thermal expansion from positive constituents, and electrical metamaterials with unusual direction and sign of the Hall voltage.

MM 25: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and Deformation I

Time: Tuesday 10:15–11:30 Location: BAR 205

Topical Talk MM 25.1 Tue 10:15 BAR 205

Atomistic Studies on the Role of Interface Curvature on Deformation and Failure of Interface-Controlled Materials — •Erik Bitzek — Department of Materials Science and Engineering, FAU Erlangen-Nürnberg

Since processes like crack nucleation and intragranular propagation as well as dislocation nucleation, absorption, transmission or pinning take place at the atomic scale, atomistic simulations have played a key role in studying grain- and interphase boundaries (GBs, IPBs). However, so far most of the studies on the deformation and failure of interface-dominated materials have been performed on simulation setups with planar interfaces.

Here we give an overview on our recent atomistic studies on intergranular fracture and dislocation-interface interactions, with the focus on non-planar boundaries and more realistic GB topologies. Examples include the importance of interface curvature on the misfit dislocation network in realistic microstructures of Ni-base superalloys, studies of slip transmission through curved GBs and the overemphasis or completely suppression of deformation mechanisms in nanocrystalline samples with different degrees of GB curvature.

MM 25.2 Tue 10:45 BAR 205

Machine learning of grain boundaries for property prediction from atomic structure and insights into their atomic building blocks — •Eric Homer[1], Conrad Rosenbrock[2], Gus Hart[2], and Hunter Erickson[1] — [1]Brigham Young University, Department of Mechanical Engineering, Provo, USA — [2]Brigham Young University, Department of Physics and Astronomy, Provo, USA

Big data is a hot topic and is driving innovation in healthcare, logistics, telecommunications, and the automotive industry. It is used in materials science to search for new materials and alloys with unique combinations of properties. We present results of machine learning applied to a large dataset of grain boundaries (GBs) to predict thermodynamic and kinetic properties of materials, including GB energy, temperature-dependent mobility trend, and shear coupling. The machine learning examines the local environment of the atoms and determines similarity metrics, from which it can make predictions. Predictions of GB energy are reasonably accurate, though the accuracy of predictions for the kinetic properties of mobility and shear coupling are lower. Nonetheless, the approach makes reasonable predictions of kinetic properties based solely on the minimum energy structure of GBs. Analysis of the trends in the machine learning data also provide insight into the possible building blocks of GBs, which appear to be a finite set.

MM 25.3 Tue 11:00 BAR 205

Coupling between grain boundary sliding and migration: misorientation dependence — •Askar Sheikh-Ali — Institute of Rheotechnologies LLC, 161-1 Kozhamkulova, 050026, Kazakhstan

Grain boundary sliding behavior has been studied in zinc bicrystals with symmetric tilt boundaries slightly deviated from 123.75°<10-10>Sigma=9 coincidence misorientation. The boundaries span a narrow range of misorientation of 123.6°-131.7°. All investigated boundaries except 131.7°<10-10> boundary demonstrate coupling between grain boundary sliding and migration predicted by DSC-dislocation model. The ratio between boundary sliding and migration is almost the same for all boundaries experiencing coupling between these processes. Sliding along 131.7°<10-10> boundary is not accompanied by regular boundary migration. The transition from coupling to migration free sliding occurred at deviation angle determined by Brandon criterion and was interpreted as a transition from special to general boundaries. Within the accuracy of the experiment, the transition angle remains constant up to the maximum investigated temperature of 400°C (0.97Tm, where Tm is the melting point).

MM 25.4 Tue 11:15 BAR 205

Coupled grain boundary motion driven by elastic anisotropy in FCC Cu — •Christian Brandl — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

Shear-coupled grain boundary motion is one mechanism, where the plastic shear deformation is linked to the microstructure changes by grain growth at low homologous temperatures. The prevailing notion on the driving force on the coupled grain boundary exclusively ascribes a shear stress in the grain boundary as the driving force. Here, we present molecular dynamics simulation to demonstrate coupled grain boundary driving by elastic anisotropy for a general large-angle asymmetry grain boundary in copper. The observed mechanisms is discussed in the framework of general driving forces of interface motion as the reduction of the total free energy grain linked to the defect migration.

MM 26: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - NMR studies

Time: Tuesday 10:15–11:30 Location: IFW A

MM 26.1 Tue 10:15 IFW A

Investigation of the Li ion conduction behavior in the solid electrolyte Li10GeP2S12 by multidimensional NMR — •Marc Paulus[1], Magnus Graf[1], Peter Notten[1,4], Rüdiger-Albert Eichel[1,3], and Josef Granwehr[1,2] — [1]FZ Jülich, Institut für Energie- und Klimaforschung , D-52425 Jülich, Germany — [2]RWTH Aachen, ITMC, D-52074 Aachen, Germany — [3]RWTH Aachen, IPC, D-52074 Aachen, Germany — [4]Department of Chemical Engineering and Chemistry, TU/e, 5600 MB Eindhoven, The Netherlands

The biggest challenge to overcome in solid electrolytes is the relatively slow and still poorly understood lithium ion migration at solid electrolyte/electrode interfaces as well as at grain boundaries in solid-state electrolytes. Li10GeP2S12 is one of the best Li-ion conductors and therefore an interesting candidate as electrolyte material in Li-ion batteries. To link lithium migration mechanisms with different structural features of LGPS by correlation of spin lattice relaxation and spin alignment echo NMR a pulse sequence with two independently varied evolution times was developed. The obtained data was processed with an algorithm for discrete Laplace inversion. The resulting spin lattice-spin alignment correlation map of LGPS provided several signal components that were assigned to different morphologies and dynamic regions in LGPS. In addition, the experiment facilitated a direct distinction between relaxation-controlled and mobility-induced components in the τc distribution. Further analysis of the spectral NMR dimension in comparison with SEM and XRD measurements yielded a diverse model of lithium motion for the LGPS powder sample.

MM 26.2 Tue 10:30 IFW A

Solid-state MAS and in-situ NMR spectroscopy for studying battery systems — Wolfram Münchgesang[1], Viktor Koroteev[2], Tatiana Zakharchenko[3], Daniil M. Itkis[4], Dirk C. Meyer[1], and •Anastasia Vyalikh[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Freiberg, Germany — [2]Nikolaev Institute of Inorganic Chemistry SB RAN, Novosibirsk, Russia — [3]Department of Material Science, Moscow State University, Moscow, Russia — [4]Department of Chemistry, Moscow State University, Moscow, Russia

Current research efforts in the field of energy storage are directed towards improving cost and performance of lithium ion batteries as well as evaluating post lithium ion concepts. Deep understanding of electrochemical processes requires quantitative information on a molecular level, on the one hand, and with temporal resolution, on the other hand. In our studies we apply ex-situ analysis using high-resolution magic angle spinning (MAS) NMR in combination with in-situ NMR, in order to characterize the electrochemical intermediates and reaction products as well as to monitor the formation of solid electrolyte interface (SEI) and surface microstructures in operating cells. The NMR results demonstrate the structural transformations in lithium ion batteries based on vanadia composite and 13C-isotop enriched carbon electrodes.

MM 26.3 Tue 10:45 IFW A

^{7}Li NMR studies of lithium ion dynamics in 70Li$_2$S-30P$_2$S$_5$ materials — •Michael Haaks[1], Steve Martin[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, TU Darmstadt, Germany — [2]Department of Materials Science and Engineering, Iowa State University, Ames, USA

Rising energy demand makes it important to improve the performance of lithium ion batteries. For this purpose it is important to understand the dynamics of lithium ions, in particular, in heterogeneous materials, which are used in modern strategies for material optimization. With combination of ^{7}Li NMR spin-lattice relaxation, diffusion measurements, line-shape, and stimulated-echo analyses it is possible to investigate lithium ionic motion in wide range of time and length scales in 0.5Li$_2$S-0.5(xGeS$_2$-(1-x)GeO$_2$)[1] and 70Li$_2$S-30P$_2$S$_5$ glasses[2]. We exploit there capabilities to ascertain the effect of ceramization in 70Li$_2$S-30P$_2$S$_5$. We find that the large variety of lithium environments results in broad distributions of correlation times for the jump motion of the lithium ions. Our results for 70Li$_2$S-30P$_2$S$_5$ allow us to relate the enhancement of electronic conductivity under ceramization[3] to faster lithium ion dynamics on various length scales.

[1] Gabriel et al., Solid State Nuclear Magnetic Resonance 70, 53 (2015)

[2] Haaks et al., work in progress

[3] Mizuno et al., Advanced Materials 17, 918 (2005)

MM 26.4 Tue 11:00 IFW A

Combined DFT and solid-state NMR study of ionic mobility in Li$_4$Ti$_5$O$_{12}$ — •Simone Köcher[1,2], Andreas Garhammer[2], Hendrik Heenen[2], Magnus Graf[1], Josef Granwehr[1], Rüdiger-A. Eichel[1], Karsten Reuter[2], and Christoph Scheurer[2] — [1]IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Jülich, Germany — [2]Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool to gain detailed understanding of the ionic mobility in battery materials. Notwithstanding, experimental spectra of novel high-capacitance electrodes such as the configurationally disordered defect spinel oxide Li$_4$Ti$_5$O$_{12}$ (LTO) are highly complex. Support by independent first-principles based calculations is indispensable to achieve an unambigious interpretation. We establish a corresponding framework for ^{7}Li spin-alignment echo NMR studies of LTO by providing first-principles reference values for chemical shielding and quadrupolar coupling from density-functional theory calculations. A detailed comparison of experimental and theoretical data suggests that a local Li ion mobility faster than the experimental time resolution must have a considerable impact on the observed NMR quantities. We present first steps towards accounting for this local dynamics in the simulation of the autocorrelation function of the NMR experiment within a kinetic Monte Carlo model.

MM 26.5 Tue 11:15 IFW A

Li-ion batteries cathode materials from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials (THEOS) and NCCR-MARVEL, EPFL, Lausanne, Switzerland

Predictive modeling of the atomistic structure and electronic properties of transition-metal (TM) compounds is essential for the development of several emerging technologies. This is particularly true for materials explored as electrodes in Li-ion batteries. Unfortunately, most approximate energy functionals fail to capture the localization of electrons on TM ions during the charge/discharge transients, thus compromising the energetics of these systems and the assessment of their performance.

Hubbard-corrected DFT functionals (DFT+U) improve significantly the description of localized valence electrons and have become the standard choice to the modeling of these TM compounds when computational efficiency is required (e.g., for screening large numbers of compounds). This work shows that an extended formulation of DFT+U, including on-site (U) and inter-site (V) interactions, improves the description of mixed valence materials. Focusing on LixMPO4 (M = Fe, Mn, Ni, Co) we discuss their equilibrium structure and electronic properties in dependence of Li content. Contradicting a common practice, we provide theoretical justification to using computed interaction parameters. We also show this is crucial to reliably compare the energy of different phases, to assess the thermodynamic stability of intermediate compositions and to evaluate the voltage of the resulting battery.

MM 27: Computational Materials Modelling - Electronic structure approaches

Time: Tuesday 10:15–11:15 Location: IFW B

MM 27.1 Tue 10:15 IFW B

A Compressed-Sensing Approach to Select Accurate Atom-Centered Basis Functions for Advanced Density Functionals and Quantum Chemistry — •Niklas Menzel[1], Luca M. Ghiringhelli[1], Gitta Kutyniok[2], and Matthias Scheffler[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Technische Universität, Berlin, DE — [3]UC Santa Barbara, USA

The choice of basis sets is a crucial factor in density functional theory and quantum chemistry, determining the accuracy and computational cost of the calculation. Commonly used basis sets are not sufficiently accurate to represent the eigenfunctions for advanced exchange-correlation treatments. This leads to basis set extensions, such as the correlation-consistent basis sets by Dunning [JCP 90, 1007 (1989)]. We have developed a new approach to select basis functions based on compressed sensing (CS), a recently developed signal processing technique. CS provides a simple and efficient framework for basis set selection based on ℓ_1-norm regularization. Our CS-based approach is applicable to all atom-centered basis sets. As introductory example, we demonstrate the selection of Gaussian-type basis functions (GTO). The number of chosen contracted or uncontracted GTOs can be tuned. We calculate the total energy for atoms from H to Ar and compare the results with Dunning's correlation-consistent basis sets, which give similar results. Our new approach enables us to determine accurate basis sets for heavier atoms including d- and f-elements.

MM 27.2 Tue 10:30 IFW B

High-order path integrals made easy — •Venkat Kapil[1], Jörg Behler[2], and Michele Ceriotti[1] — [1]Laboratory of Computational Science and Modelling, Institute of Materials, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Lehrstuhl f ur Theoretische Chemie, Ruhr-Universit at Bochum, Bochum, Germany

The precise description of quantum nuclear fluctuations in atomistic modelling is possible by employing path integral techniques, which involve a considerable computational overhead due to the need of simulating multiple replicas of the system. Many approaches have been suggested to reduce the required number of replicas. Among these, high-order factorization of the Boltzmann operator are particularly attractive for high-precision and low-temperature scenarios. Unfortunately, to date several technical challenges have prevented a widespread use of these approaches to study nuclear quantum effects in condensed-phase systems. Here we introduce an inexpensive molecular dynamics scheme that overcomes these limitations, thus making it possible to exploit the improved convergence of high-order path integrals without having to sacrifice the stability, convenience and flexibility of conventional second-order techniques. The capabilities of the method are demonstrated by simulations of liquid water and ice, as described by a neural-network potential fitted to dispersion-corrected hybrid density functional theory calculations.

MM 27.3 Tue 10:45 IFW B

New Dynamical Mean-Field Theory capabilities in CASTEP — •Evgeny Plekhanov[1], Vincent Sacksteder[2], Phil Hasnip[3], Matt Probert[3], Stewart Clark[4], Cedric Weber[1], and Keith Refson[2] — [1]Department of Physics, Faculty of Natural and Mathematical Sciences King's College London Strand, London, WC2R 2LS, UK — [2]Department of Physics, Royal Holloway University of London, Egham, Surrey TW20 0EX, UK — [3]Department of Physics, University of York, Heslington, York YO10 5DD, UK — [4]Department of Physics, University of Durham, Durham DH1 3LE, UK

We present the first implementation of Dynamical Mean-Field Theory in UK's major ab-initio code CASTEP [1]. This implementation: i) is modular; ii) allows great flexibility in choosing local basis set for downfolding/upfolding of self-energy; iii) permits wide choice of impurity solvers (including external solver libraries); and iv) gives the user a possibility to use several self-consistency schemes and calculate total energy and forces. We explain in details the theoretical framework used. We benchmark our implementation on several strongly-correlated insulating systems with d- and f-shells: γ-Ce and Ce_2O_3 by using Hubbard I and CTHYB-QMC solvers. Our results appear to be in excellent agreement with the reference data published previously in the literature [2,3,4].

[1] E. Plekhanov, et al. in preparation (2016). [2] L. Pourovskii, et al. Phys. Rev. B 76, 235101 (2007). [3] B. Amadon, et al. Phys. Rev. B 77, 205112 (2008). [4] J. Kuneš, et al. Phys. Rev. Lett. 99, 156404 (2007).

MM 27.4 Tue 11:00 IFW B

Analytical continuation of Green's functions using Padé approximants — •Johan Schott — Uppsala University, Uppsala, Sweden

A critical step to obtain physical observables for many Green's function based methods is the ill-posed analytical continuation problem. We propose to remedy the known instability problems of the Padé approximant method by averaging several continuations, using different number of Padé approximant coefficients and input points. In our article [Phys. Rev. B 93, 075104 (2016)] we also show including negative Matsubara frequencies further improves the peak resolution possibility. The importance of high numerical precision, even for very noisy input data, is systematically presented. Lastly, the presented method is compared to a number of other analytical continuation methods, showing good performance.

MM 28: Transport I - atomic transport

Time: Tuesday 10:15–11:45 Location: IFW D

MM 28.1 Tue 10:15 IFW D

Volume diffusion in high-entropy Al_xCoCrFeNi alloys — •Josua Kottke[1], Simon Trubel[1], Matthias Wegner[1], Louis J. Santodonato[2], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Unversity of Münster, Germany — [2]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, USA

High-entropy alloys, i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as potential structural materials due to their favorable mechanical and physical properties, especially at elevated temperatures. In the present study, the tracer diffusion of Cr, Co, Fe, and Ni is measured in the Al_xCoCrFeNi alloys at 1000°C and 1100°C applying the ^{51}Cr, ^{57}Co, ^{59}Fe and ^{63}Ni radioisotopes, respectively. The addition of Al to the CoCrFeNi FCC alloy is known to induce the appearance of a two-phase, FCC+BCC, microstructure which is examined using EBSD and EDX analyses. A correlation between the phase decomposition tendency and the tracer diffusivities of constituent elements is discussed.

MM 28.2 Tue 10:30 IFW D

Novel method to predict effects of structural changes on energy barriers in NASICON materials — •Kaustubh Bhat, Stefan Blügel, and Hans Lustfeld — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Among ionic conductors, NASICON [1] materials are receiving renewed attention because of their compositional diversity, particularly for large-scale energy storage applications. We first use the Nudged Elastic Band (NEB) method for calculating the energy barrier for sodium ion transport in $Na_6Sc_4\,(PO_4)_6$. Small changes in structure cause changes in the energy barrier. We model this using the second-order force constant matrices at the ground state and at the saddle point, and have developed a method to calculate the new ground state, the new saddle point state and thus the new energy barrier without performing a new NEB calculation. We propose a method to find the new force constant matrices and their corresponding eigenvalues at the new extrema. We validate this method using several materials eg. $Na_6Sc_4\,(SiO_4)\,(PO_4)_5$ [2].

[1] H.Y.P. Hong, Mat. Res. Bull. **11**, 173-182 (1976).
[2] M. Guin and F. Tietz, J. Power Sources **273**, 1056 (2015).

MM 28.3 Tue 10:45 IFW D

Chemical and tracer diffusion in the Fe-Ga binary couple — •Bengü Tas-Kavakbasi[1], Aloke Paul[2], Igor Stanislavovich Golovin[3], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Department of Materials Engineering, Indian Institute of Science, Bangalore, India — [3]National University of Science and Technology "MISiS", Moscow, Russia

In the present study, Manning's "sandwich interdiffusion" approach is applied to the Fe-Ga binary system and the interdiffusion measurements are directly combined with a tracer diffusion experiment. The ^{55}Fe radioisotope is deposited on the outer surfaces of a Fe-8Ga/Fe-24Ga interdiffusion couple (the concentrations are given in at.%) and on the initial interface between the two alloys. The couple was subsequently annealed at 900°C. The interdiffusion coefficient at 900°C is determined using electron probe profiling and the standard Sauer-Freise analysis. A strong composition dependence of the interdiffusion coefficient was found and its dependence on the molar volume is evaluated. The composition dependence of the ^{55}Fe tracer diffusion coefficient in the Fe-8Ga/Fe-24Ga interdiffusion couple has been determined, too.

MM 28.4 Tue 11:00 IFW D

Diffusion and ionic conductivity from ab initio non-equilibrium molecular dynamics — •Sergei Simak — IFM, Linköping University, SE-58183 Linköping, Sweden

Even fast diffusion and ionic conductivity in solids are too slow for studies from accurate ab initio equilibrium molecular dynamics (MD). The use of the nonequilibrium color-diffusion algorithm allows one to substantially speed up the simulations. Our recent implementation of the algorithm has been applied to the problem of oxygen diffusion and ionic conductivity in doped ceria, a promising electrolyte material for intermediate temperature solid oxide fuel cells (IT-SOFCs). The application of the methodology speeds up the simulated oxygen transport by a factor 60 compared with standard equilibrium MD. The calculated conductivity values agree with the available experimental data, and the experimental temperature trend is well reproduced [1-2]. The developed methodology might be useful for a large number of problems related to diffusion.

REFERENCES.

1. J. Klarbring, O. Yu. Vekilova, J. O. Nilsson, N. V. Skorodumova, and S. I. Simak, "Ionic conductivity in Sm-doped ceria from first-principles non-equilibrium molecular dynamics", Solid State Ionics, 296, 54 (2016).
2. J. O. Nilsson, O. Yu. Vekilova, O. Hellman, J. Klarbring, S. I. Simak, and N. V. Skorodumova , "Ionic conductivity in Gd-doped CeO2: Ab initio color-diffusion nonequilibrium molecular dynamics study", Phys. Rev. B 93, 024102 (2016).

MM 28.5 Tue 11:15 IFW D

Grain boundary diffusion and segregation of ^{57}Co in high-purity copper: Radiotracer measurements in B- and C-type diffusion regimes — •Daniel Gaertner, Gerhard Wilde, and Sergiy Divinski — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Grain boundary diffusion of ^{57}Co in high-purity polycrystalline copper is investigated using the radiotracer technique in Harrison's B- $(850 - 1150$ K) and C-type $(550 - 950$ K) kinetic regimes. The triple product $P = s \cdot \delta \cdot D_{\mathrm{gb}}$ (s is the segregation factor and δ the grain boundary width) and the grain boundary diffusion coefficient D_{gb} of Co in Cu are determined to obey the Arrhenius laws with the activation enthalpies of $Q_{\mathrm{gb}} = 66.2$ kJ/mol and $H_{\mathrm{gb}} = 100.9$ kJ/mol, respectively. Using the experimental estimate of δ, $\delta \cong 0.5$ nm, Co is found to segregate strongly at Cu grain boundaries and the corresponding segregation factor follows an Arrhenius dependence with the segregation enthalpy of $H_s = -34.7$ kJ/mol . Co-diffusion experiments with the ^{57}Co and ^{110m}Ag isotopes support a 'sub-interface'-type of grain boundary segregation of Co in Cu.

MM 28.6 Tue 11:30 IFW D

Modeling hydrogen diffusion in amorphous and polycrystalline thin films of tungsten trioxide — •Simon Burkhardt[1], Matthias Thomas Elm[1,2], and Peter Jens Klar[1] — [1]Heinrich-Buff-Ring 16, 35392 Giessen — [2]Heinrich-Buff-Ring 17, 35392 Giessen

The mandatory development of efficient energy management also will advance the commercialization and industrialization of electrochromic fenestration. Most of these devices are based on the electrochromic behavior of thin films such as tungsten trioxide (WO_3) induced by reversible insertion and extraction of ions and electrons into the films. A consistent fundamental understanding of the coloration processes is still lacking up to now but is needed to systematically enhance device performance and to increase their cyclability. To elucidate the transport behavior of protons and electrons in WO_3 thin films, we performed spatially and temporally resolved in situ transmission measurements on lithographically structured samples during electrochemical hydrogen insertion into amorphous and polycrystalline thin films. The experimental results show a significant influence of film morphology on lateral hydrogen diffusion and are compared with different simulations of theoretical models. These models are based on one dimensional diffusion problems in different continuous media and describe the experimental data qualitatively very well.

MM 29: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III

Time: Tuesday 10:30–13:00 Location: GER 38

Invited Talk MM 29.1 Tue 10:30 GER 38

Including spin effects in the strong-coupling limit of DFT — •Paola Gori-Giorgi[1], Juri Grossi[1], Derk Pieter Kooi[1], Klaas Giesbertz[1], Michael Seidl[1], Aron Cohen[2], and Paula Mori-Sanchez[3] — [1]Vrije Universiteit Amsterdam, The Netherlands — [2]University of Cambridge, UK — [3]Universidad Autonoma de Madrid, Spain

The exact strong-coupling limit of density functional theory (DFT) reveals a different mathematical structure with respect to the one of traditional approximations for the exchange-correlation (xc) functional: instead of the local density, local density gradients, or quantities related to the Kohn-Sham orbitals, some integrals of the density appear in this limit. In the recent years, xc functionals directly inspired to this mathematical structure have been constructed and implemented in an efficient way. However, the leading terms (exact or approximate) in the strong-coupling limit of DFT are intrinsically semiclassical and, as such, do not incorporated the spin dependence. In this talk, I will present the first study on the incorporation of the spin-dependence in the exact strong-coupling limit in simple one-dimensional cases. I will then discuss approximations for our findings and routes to the construction of spin-dependent xc functionals for strong coupling. Comparison with exact calculations for the Hohenberg-Kohn functional in the strong-coupling regime confirms the accuracy of our expressions for the leading terms.

MM 29.2 Tue 11:00 GER 38

Strong correlation from the Random Phase Approximation and beyond — •Thomas Olsen and Kristian Thygesen — Department of Physics, Technical University of Denmark

We assess the performance of the Random Phase Approximation (RPA) for strongly correlated systems and discuss different routes to venture beyond RPA. It is well-known that RPA reproduces the dissociation curve of molecular H2 correctly and thus accurately captures the strong static correlation inherent in the dissociation limit. It is thus natural to ask whether RPA is able to describe the strongly correlated Mott insulators as well. In particular, the accurate description of antiferromagnetic systems is complicated by the fact that the magnetic order often emerges from a detailed interplay between direct exchange and super-exchange couplings, which are respectively exchange and correlation effects. Whereas DFT+U, semi-local and hybrid functionals are often capable of describing either exchange or super-exchange accurately, RPA is shown to give an accurate account of both. We will finally show that RPA can be improved by either including non-local kernel in the framework of TDDFT or including electron-hole interactions in the irreducible response function. Only the latter approach improves the description of strong correlation, whereas the former approach improves atomization energies significantly compared to RPA.

MM 29.3 Tue 11:15 GER 38

Surface and adsorption energy calculations within the random phase approximation — •Per Schmidt and Kristian Thygesen — Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The application of density functional theory (DFT) to the calculation of adsorption and surface energies is ever increasing and as a theory, it has the potential to e.g. guide experiments in the search of better catalysts. However, a previous study[1] shows that with standardly used semi-local functionals, DFT is not able to accurately predict surface and adsorption energies simultaneously. By tuning the functional, either the predicted surface or adsorption energies can be improved at the expense of the other. For a few cases however, it has been shown[1] that the many-body approach, the random phase approximation (RPA), yields both excellent surface and adsorption energies.

In this work we expand the use of the RPA method to eight adsorption reactions over 20 transition metal surfaces using the electronic structure code GPAW. We report the difference in surface and adsorption energies compared with the standard DFT functionals: PBE, RPBE and BEEF-vdW. We find that RPA does in general predict less stable surfaces, in better agreement with experiments and the average change in adsorption energies varies between ± 0.5 eV. The RPA values could be used to guide construction of new density-functionals aimed at improving surface science calculations.

[1] L. Schimka, J. Harl, A. Stroppa, A. Grüneis, M. Marsman, F. Mittendorfer, and G. Kresse, Nature Materials 9, 741 (2010).

MM 29.4 Tue 11:30 GER 38

Large-scale cubic-scaling RPA correlation energy calculations using a Gaussian basis — •Jan Wilhelm and Jürg Hutter — University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

The random phase approximation (RPA) for computing the electron correlation energy has emerged as an accurate tool for predicting the properties of molecules and condensed phase systems. RPA combines a number of attractive features, most importantly that long-range van der Waals interaction is included, in contrast to semilocal density functionals. The drawback connected with RPA is the computational cost: For canonical implementations of RPA, the numerical effort grows as quickly as $O(N^4)$ with the system size N. We present an algorithm for computing the RPA correlation energy in a Gaussian basis requiring $O(N^3)$ operations and $O(N^2)$ memory. The cubic-scaling RPA method is based on the resolution of the identity (RI) with the overlap metric, a reformulation of RI-RPA in the Gaussian basis and imaginary time as well as the use of sparse linear algebra. We report a massively parallel implementation which is the key for the application to large systems. As first benchmark of the method, we show the RPA correlation energy of thousands of water molecules in a high-quality cc-TZVP basis. For a comparison, the canonical RPA method is restricted to 500 water molecules using the whole Piz Daint supercomputer for two hours. Our RPA algorithm enables the application of RPA to large systems where van der Waals interactions play an important role, e.g. for predicting the adsorption energy of large molecules on surfaces.

MM 29.5 Tue 11:45 GER 38

Semi-local exchange functionals showing ultranonlocal response: the hope to replace exact exchange — •Thilo Aschebrock and Stephan Kümmel — Theoretical Physics IV, University of Bayreuth, D-95440 Bayreuth, Germany

The widespread success of Density Functional Theory (DFT) is based on a favorable ratio of accuracy to computional cost, especially with semi-local approximations to the exchange-correlation energy. However, functionals such as the local density approximation (LDA), generalized-gradient approximations (GGA) or meta-generalized-gradient approximations (meta-GGA), typically miss important exact exchange features related to the derivative discontinuity. These are essential for accurately describing long-range charge transfer processes. The electrical response of molecular chains, which is dramatically overestimated by local and semi-local density functionals, is a prime example. The key to its correct description is a term in the Kohn-Sham exchange potential that counteracts the external field and has been named "ultranonlocal". We here present how these field-counteracting properties can be incorporated into semi-local DFT on the meta-GGA level. Thereby we show that by utilizing the kinetic-energy-density, it is possible to model ultranonlocal effects in the Kohn-Sham potential by virtue of a semi-local energy expression.

MM 29.6 Tue 12:00 GER 38

(De)stabilizing dispersion interactions via external electric charges — •Andrii Kleshchonok[1] and Alexandre Tkatchenko[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

Van der Waals (vdW) or dispersion interactions play a central role in the structure, stability, and reaction mechanisms in large variety of molecules and materials. However, in many situations of interest in material science and biophysics, vdW interactions should account for the coupling with external (in)homogeneous electric fields. In this work we address the effect of external static charge field on long-range electron correlations. By using the quantum Drude oscillator model, we derive analytical expressions of the charge induced dipole-quadrupole dispersion energy, that is accounted neither in standard DFT methods, nor in popular vdW correction schemes. Analysing the scaling laws of this dispersion term, we conclude that positive charge stabilizes dispersion interactions, while a negative charge has an opposite effect. Benchmark over S22 molecular dataset estimates the induced dispersion to be in the range of 20-300 % of conventional electrostatic energy. Our findings could have broad potential implications, including exfoliation of 2D materials, chemical reaction rates in charged droplets, and biological membranes.

MM 29.7 Tue 12:15 GER 38

An optimisability proof for self-consistent constrained DFT, and its implications for constraint-based self-interaction error correction — Glenn Moynihan[1], Gilberto Teobaldi[2,3], and •David D. O'Regan[1] — [1]School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland. — [2]Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, U.K. — [3]Beijing Computational Science Research Center, China.

We develop the connection between constrained DFT energy derivatives and response functions, providing a rigorous assessment of the uniqueness and character of cDFT stationary points while accounting for electronic interactions and screening [1]. In particular, we provide a non-perturbative proof that stable stationary points of linear density constraints occur only at energy maxima with respect to their Lagrange multipliers, generalizing the proof of Ref. [2]. We demonstrate that multiple solutions, hysteresis, and energy discontinuities may occur in cDFT, and we provide necessary conditions for the optimizability of multi-constraint cDFT. We show that the applicability of cDFT in automating symmetry-preserving self-interaction error corrections is limited by a fundamental incompatibility with non-linear constraints. We circumvent this by utilizing separate linear and quadratic correction terms, which may be interpreted either as distinct constraints, each with its own Hubbard U type Lagrange multiplier, or as the components of a generalized, two-parameter DFT+U functional [3]. [1] Phys. Rev. B **94**, 035159 (2016). [2] Phys. Rev. A **72**, 024502 (2005). [3] Phys. Rev. B Rapid Comms., Accepted (2016), arXiv:1608.07320.

MM 29.8 Tue 12:30 GER 38

Density-based local hybrid functional for interfaces — •Pedro Borlido[1], Silvana Botti[1], and Miguel Marques[2] — [1]Institu für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743, Jena, Germany — [2]Instiut für Physik, Martin-Luther-Universität Halle Wittenberg, D-06099 Halle, Germany

Hybrid functionals in density functional theory have become the state-of-the-art for the calculation of electronic properties of solids. The key to their performance is how and in which amount a part of Fock exchange is mixed with semi-local exchange-correlation functionals. We propose here a material dependent and local mixing parameter which is a functional of the electron density alone, through an estimator of the local dielectric function inspired by the work done in *Phys. Rev. B* 83, 035119 (2011). This new functional is by construction an approximation of the GW self-energy and it enables therefore calculations of quasiparticle energy levels of comparable quality as GW, but at the reduced cost of a hybrid density functional. In contrast with other recent self-consistent schemes for the mixing parameter, our approach does not require to calculate the dielectric function and leads to a negligible increase of the computation time.

MM 29.9 Tue 12:45 GER 38

On the hunt for better functionals in DFT: a new quantum embedding scheme — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new systematic technique to derive functionals for standard density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

Not only the DMET scheme is improved by the uniqueness of the density-potential mapping, the proposed density-embedding also allows for finding accurate Kohn-Sham potentials. Moreover, unlike in usual DFT, we can systematically improve the description by increasing the size of the active space.

We show benchmark results of our method for molecules in 1D.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

MM 30: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and Deformation II

Time: Tuesday 11:45–13:00 Location: BAR 205

MM 30.1 Tue 11:45 BAR 205

Low angle grain boundaries induced buckling in nanoscale copper films — •Xiaopu Zhang[1], Jian Han[2], David Srolovitz[2], and John Boland[1] — [1]CRANN, Trinity College Dublin, Dublin 2, Ireland — [2]Department of Materials Science and Engineering, University of Pennsylvania, 3231 Walnut St., Philadelphia, PA 19104 USA

Scanning tunneling microscopy is used to study the grain boundaries that emerge at the surface of nearly coplanar copper nanocrystalline films with (111) surface orientations. At symmetric low angle grain boundaries the film is found to buckle so as to form valleys comprised of dissociated edge dislocations and ridges where dislocations have recombined. Geometry analysis shows that buckling is induced by the out-of-plane grain rotation driven by the favorable energy of dislocation-dissociation, and confirmed by simulations. Due to the symmetry of the FCC slab, both the type of emergent grain boundaries (dissociated or recombined) and the film buckling sense are forced to toggle whenever grain boundaries shift direction by 60o, producing a novel buckling pattern. These results indicate that it is impossible to form perfectly flat two dimensional nanoscale films of copper and indeed other metals that exhibit low dislocation-dissociation energies.

MM 30.2 Tue 12:00 BAR 205

Tensorial elastic properties and stability of interface states associated with $\Sigma5(210)$ grain boundaries in Ni$_3$(Al,Si) — •Martin Friák[1,2], Monika Všianká[2,1], David Holec[3], and Mojmír Šob[2,1,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GBs) represent one of the most important types of defects in solids. They are challenging for theoretical studies because of their distorted atomic structure. We use *ab initio* methods to assess tensorial elastic properties of interface states associated with GBs. Focusing on the $\Sigma5(210)$ GBs in Ni$_3$Al intermetallics as a case study, we evaluate the mechanical stability of the interface states by checking Born-Huang's stability criteria. The elastic constant C_{55} is found three-/five-fold lower than in the bulk and, as a result, the mechanical stability of interface states is reduced. The tensorial elasto-chemical complexity of the interface states is demonstrated by a high sensitivity of elastic constants to the GB composition. In particular, we study elasticity changes induced by Si atoms segregating into the atomic layers close to the GBs and substituting Al atoms. If wisely exploited, our study paves the way towards solute-controlled design of GB-related interface states with tailored stability and/or tensorial properties.

MM 30.3 Tue 12:15 BAR 205

Grain boundary strain accommodation mechanisms in ultrafine-grained Pd — •Yulia Ivanisenko[1], Nariman A. Enikeev[2], and Kejing Yang[3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, 450000 Ufa, Russia — [3]Robert Bosch GmbH, AE/EAI2, D71701 Schwieberdingen, Germany

The role of non-crystallographic deformation modes such as grain boundary sliding and rotation in plasticity of ultrafine-grained materials (UFG) is still a matter of discussion. In general, it is assumed that such strain accommodation is considerable at grain sizes in the range of a few tens of nanometers while for the larger grains dislocation-based mechanisms operate. In situ SEM compression test was performed on UFG Pd sample with a mean grain size of 135 nm and orientations of statistically sound sampling of grains were monitored. In order to separate the effects related with dislocation slip, the modeling of the evolution of grain orientations under compression using the methods of crystal plasticity simulation were performed. The analysis of the results shows that grain boundary sliding and non-crystallographic grain rotations contribute considerably to the plasticity of UFG materials. The grains tend to slide and to rotate in a group mode, which testifies to collective character of grain boundary deformation mechanisms in UFG Pd. It was proposed that such grain rotations provide a mechanism for the accommodation of the strain incompatibility between neighboring grains arising during straining.

MM 30.4 Tue 12:30 BAR 205

Energetics of deformed As, Sb and Bi and local deformation of overlayers at interfaces with various substrates — Martin Zouhar[1] and •Mojmir Sob[1,2,3] — [1]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [3]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We present a comprehensive density-functional theory study of total energy and structural properties of As, Sb and Bi in their A7 ground-state structure and in the bcc, fcc and simple cubic (sc) modifications. We also investigate continuous structural transitions between these structures. The total energies of deformed structures are displayed in contour plots as functions of selected structural parameters and/or atomic volume; these plots are then used for understanding and interpreting structural parameters of As, Sb and Bi overlayers on various substrates. Our calculated values of lattice parameters for (0001) thin films of Bi on Si(111) and Ge(111) substrates agree very well with available experimental data. In analogy with that, we suggest to investigate (0001) overlayers of As on Ti(0001), Co(0001), Zn(0001) and Rh(111) substrates, of Sb on C(0001), Zn(0001), Al(111), Ag(111) and Au(111) substrates and of Bi on Co(0001), Al(111), Rh(111), Ba(111) and Pb(111) substrates. For these cases, we also predict the lattice parameters of the films. A large part of our results are theoretical predictions which may motivate experimentalists for a deeper study of these systems.

MM 30.5 Tue 12:45 BAR 205

Deformation behavior in multilayered thin films with different interface structures under sliding contact — •Ankush Kashiwar[1], Zhao-Ping Luo[2], Ruth Schwaiger[1,3], and Christian

Kübel[1,3] — [1]Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Shenyang National Laboratory for Materials Science, Shenyang 110016, China — [3]Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

The presented study aims at investigating the deformation structure under sliding contact in multilayered systems with different interface structures. Cyclic sliding experiments were performed on sputtered nanocrystalline metallic multilayers with semi-coherent (Au/Cu) and incoherent (Cu/Cr) interfaces. The deformed microstructure was investigated using automated crystal orientation mapping (ACOM) in a transmission electron microscope. It is revealed that Au/Cu multilayers with a high density of twins deform by de-twinning and grain growth with a simultaneous vortex-like co-deformation and mechanical intermixing between Au and Cu layers. In case of Cu/Cr multilayers, a significant grain growth is observed in all the Cu layers and the grain size increases with the increasing number of loading cycles, whereas there is no noticeable change in the grain sizes in the Cr layers. Unlike Au/Cu multilayers, the phase maps show sharp boundaries between Cu and Cr layers, indicating no intermixing between the layers.

MM 31: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Structure - property relationships I

Time: Tuesday 11:45–12:45 Location: IFW A

MM 31.1 Tue 11:45 IFW A

Hierarchically Structured Electrode Materials for Lithium-Ion Batteries — •Michael Fischer, Xiao Hua, Preston Sutton, and Ullrich Steiner — Adolphe Merkle Institute, Chemin des Verdiers 4, 1700 Fribourg, Switzerland

We present a facile synthetic approach for the fabrication of hierarchically structured electrode materials for lithium-ion batteries. Amphiphilic block copolymers are known to form well-defined morphologies on a mesoscale. By confining sol-gel chemistry to one of the blocks of the polymer these structures can be transferred to various inorganic materials, including functional materials that find use in batteries. Blending the sol-gel precursor/block copolymer mixture with a homopolymer induces phase separation and leads to structure formation on a secondary (micrometre) scale. Following this method, we synthesized mesoporous microspheres of TiO2 and Li4Ti5O12/C as anode materials and hollow LiFePO4/C nanospheres as a cathode. These compounds suffer from intrinsically low ionic and electronic conductivities but are of great interest due to their inherent stability and safety. The aforementioned morphologies circumvent this drawback by providing shortened solid-state diffusion distances, facilitating ionic transport. In addition, we can tune the mesopore size by employing block copolymers of different chemical composition and molecular weight. Studying the relationship between pore size and electrochemical performance enables us to identify design principles for the optimization of electrode architectures.

MM 31.2 Tue 12:00 IFW A

Comparison of different thin-film solid-state battery systems — •Susann Nowak, Juliane Mürter, and Guido Schmitz — Heisenbergstr. 3, 70563 Stuttgart

Different systems of thin-film batteries will be compared in respect to their suitability of being used as a reasonable combination of materials in an all-solid-state battery. As the cathode lithium iron phosphate, lithium cobalt oxide and lithium manganese oxide are compared. The used electrolyte is LiPON and as the anodes tin, silicon and lithium are tested. All cells are prepared by ion-beam sputtering resulting in an overall thickness of one micrometer or less for the whole cell. Electrochemical and TEM investigations are used to evaluate the changes at the interfaces and in the electrodes during cycling and to show mechanisms of capacity loss in the system. The behavior of lithium iron phosphate is very different from the one of lithium cobalt oxide when covered with LiPON. The capacity of the LFP covered with LiPON is exponentially increasing with the temperature and reaching its theoretical value at around 70°C. In the case of all-solid-state batteries with other anodes than lithium, the capacity becomes dependent on the chosen balancing ratio of the cells.

MM 31.3 Tue 12:15 IFW A

Ion transport and phase transformation in thin film LiFePO4 intercalation electrodes — •Guido Schmitz[1], Fabian Wunde[2], and Frank Berkemeier[2] — [1]Institut für Materialwissenschaft, Univ. Stuttgart, Heisenbergstr. 3, 70569 Stuttgart — [2]formerly: Institut für Materialphysik, Univ. Münster

Thin film battery materials have an important potential to be applied in all-solid-state batteries. From the view point of physics, they offer a clearer model geometry than the usual particle-binder-compound electrodes. The phase diagram of LiFePO4 predicts a phase separation in the Li intercalation. However, it is controversial whether phase separation might be suppressed in nanosystems due to elastic or kinetic constraints.

We study the intercalation kinetics of thin films under variation of the intercalation rate over more than 4 orders of magnitude. Also the layer thickness has been systematically varied. We show i) that the miscibility gap of the bulk system is essentially understood by elastic interaction, ii) that nanometric thin films clearly reveal phase separation and therefore undergo significant plastic relaxation, iii) that the grain boundaries represent fast transport paths with the electrochemical characteristics of an ion-conductor and iv) how the classic Randles-Sevcik analysis has to be modified in the case of a phase-separating material to derive proper diffusion coefficients.

MM 31.4 Tue 12:30 IFW A

First-Principles Calculations on Structure and Reactivity of Amorphous LiPON — •Sabrina Sicolo and Karsten Albe — Institute of Material Science, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Despite their increasing popularity as solid electrolytes, the structure/property relationship of Lithium Phosphorus Oxynitrides has not yet been clarified. Theoretical work offers an invaluable insight into the atomistic properties of solids, provided the availability of valid structural models. The simulation of glassy structures represents a main challenge from a computational point of view, and is further complicated by their non-trivial composition. In this contribution, a new approach to the ab-initio simulation of amorphous structures of virtually any desired composition is described. A realistic composition has been suggested by experiments recently conducted by academic partners. The defect thermodynamics of LiPON suggests its instability against metallic lithium. [1] The formation of a solid-electrolyte interphase (SEI) at this interface has been recently observed and quantified experimentally. Following up on this result, the interfacial structural and electronic properties have been investigated with a special focus on reactivity. This work does not only describe a novel approach to the simulation of a more realistic electrolyte, but also provides unprecedented insights, supported by experimental results, into its stability and reactivity under operational conditions.

[1] S. Sicolo, K. Albe, J. Power Sources 331, 382-390 (2016).

MM 32: Microstructure and Phase Transformations - detection methods

Time: Tuesday 11:45–13:15 Location: IFW B

MM 32.1 Tue 11:45 IFW B

In situ investigation of the Microwave-Assisted Solvothermal Synthesis process by Small-Angle X-ray Scattering — •Eike Gericke[1], Robert Wendt[1], Armin Hoell[2], Dragomir Tatchev[3], Simone Raoux[2], and Klaus Rademann[1] — [1]Humboldt-Universität zu Berlin, Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Bulgarian Academy of Sciences, Sofia, Bulgaria

Microwave-assisted solvothermal syntheses (MWASS) improve well-established solvothermal syntheses for the preparation of monodisperse and crystalline metal and metal oxide nanoparticles. MWASS allows a precise control of pressure and temperature inside a sealed reaction vessel. The advantage in contrast to conventional heating is the efficient internal heating by direct coupling of MW energy into the precursor solution, allowing high heating rates with small thermal gradients. Hence, the reaction times are decreased significantly and can be described by the Arrhenius law. Understanding the reaction mechanisms inside a MWASS reactor is important to influence and optimize the reaction process accordingly. The reaction kinetics are in a scale of seconds. So, the nucleation and growth processes taking place in a sealed high-pressure reactor have to be monitored under extreme conditions. A sample environment, elegant adjusted to these conditions will be presented, usable for in situ SAXS. Extension by WAXS and XAS or UV-vis and Raman are possible. It resists harsh chemical conditions and pressures above 30 bar. Results from experiments at Elettra and ESRF will be presented allowing unique insights in the particles growth mechanisms during a MWASS.

MM 32.2 Tue 12:00 IFW B

Time resolved diffraction on cooling of Ti-Fe alloys solidified from different undercooling levels — •Olga Shuleshova[1], Ivan Kaban[1], Dirk Holland-Moritz[2], Jan Gegner[2], Junhee Han[1], Norbert Mattern[1], and Jürgen Eckert[3] — [1]Institute for Complex Materials, IFW Dresden, Germany — [2]Institute of Materials Physics in Space, DLR, Cologne, Germany — [3]Montan-University Leoben, Austria

Melt undercooling is a necessary precondition to begin solidification. With help of the containerises processing, realised in different levitation techniques, undercoolings of the order of several hundreds degrees are easily achieved in many pure metals as well as in metallic alloy systems. With increasing undercooling a profound effect of solute trapping have been observed in alloys. Time resolved diffraction of synchrotron X-rays on levitated metallic droplets allows to quantitatively analyse the level of supersaturation present in the sample immediately after solidification and trace its further evolution as sample is cooled down. Applied to the Ti-Fe system this method have shown a non-intuitive results due to coupling with other effect of undercooling - the microstructure refinement. Financial support by DFG under project No. SH 578/1-1 is gratefully acknowledged.

MM 32.3 Tue 12:15 IFW B

Positron-μm-beam for the Coincident Doppler Broadening Spectrometer at NEPOMUC — •Thomas Gigl, Marcel Dickmann, Markus Reiner, Benjamin Rienäcker, Matthias Thalmayr, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The positron beam facility NEPOMUC (Neutron induced Positron Source Munich) at the neutron source FRM II provides a monoenergetic positron beam with high intensity of 10^9 moderated positrons per second. A new CDB spectrometer was set into operation which enables defect studies by conventional Doppler broadening spectroscopy (DBS) and element-specific measurements with coincident DBS (CDBS) at the near surface and in the bulk of a sample with a positron implantation energy of up to 30 keV. According to first spatially resolved measurements the CDB Spectrometer provides a lateral resolution of 200 μm. With an additional 100 nm thin Ni(100) remoderation foil in transmission geometry a resolution of 50 μm could be measured. In order to achieve a high yield of re-emitted moderated positrons, the Ni foil has to be annealed and surface contaminations such as C and O have to be removed. For this purpose the foil was heated to about 400°C in a H-atmosphere of about 10^{-3} mbar. After this procedure and cooling down to room temperature, the moderation efficiency of the Ni(100) foil could be measured to about 10%. Financial support by BMBF (project no. 05K10WOB) is gratefully acknowledged.

MM 32.4 Tue 12:30 IFW B

The lattice strain in single-phase high-entropy alloys — •Junhee Han[1], Pramote Thirathipviwat[1,2], Jens Freudenberger[1], Jozef Bednarcik[3], Norbert Mattern[1], and Thomas Gemming[1] — [1]IFW Dresden, PO Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — [3]DESY Photon Science, Notkestraße 85, 22607 Hamburg, Germany

The formation of single-phase solid solutions in high-entropy alloys (HEAs) consisting of multiple principal elements has led to the proposition that the lattices of HEAs must be severely distorted. Severe lattice distortion constitutes one of the key features characterizing high-entropy alloys and their enhanced mechanical properties. However, quantitative determination of the lattice distortions have only rarely been investigated. In order to address this issue, we employed means of X-ray diffraction (XRD) studies to investigate both long-range and atomic-scale distortions in the fcc-structured HEA and its binary, ternary and quaternary subsystems. The long-range and the local lattice strain were determined from the peak broadening analysis of X-ray diffraction and pair distribution functions (PDF). Particular attention is paid to the relative difference in the lattice distortions between the HEA and their subsystems including unary fcc-Ni. The HEA exhibited only slight changes in the long-range and local lattice strain compared to those of the subsystems. The results in this study indicate that the lattice strains in the equiatomic HEA is only slightly distorted away from the average fcc structure.

MM 32.5 Tue 12:45 IFW B

Imaging and kinetics of MgH2 formation — •Efi Hadjixenophontos[1], Manuel Roussel[1], Toyoto Sato[2], Patrick Stender[1], Shin-ichi Orimo[2,3], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft (IMW) University of Stuttgart, Heisenbergstrasse 3, 70569 Stuttgart GERMANY — [2]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 JAPAN — [3]WPI-Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 JAPAN

Storage in metal hydrides is presented as one of the solutions to solve the hydrogen storage problem. MgH2 is one of the ideal materials, studied intensively for the hydrogen fuel based economy. This reversible system has however some drawbacks. Hydrogen and Mg are strongly bonded by a H bond, and this makes the stable compound unpractical for commercial use. During this work Mg thin films will enable us to monitor the growth process of the hydride and study the mechanism of hydride formation. Pd is used as a catalyst coating for decreasing the pressure and temperature of hydrogenation to 5bars and 100°C. The hydride formation has been followed by in-situ XRD characterization. Microscopic imaging of the co-existence of MgH2 and Mg is presented by SEM and TEM. The microstructure change is clearly visible in the micrographs, despite the fact that electron microscopy damages the hydride phase. These combined techniques are a great way to follow the kinetics of hydride formation within the layer,and study further the diffusion coefficients and mechanism of hydrogenation at 200°C and 300°C and at different pressures (1-100bars).

MM 32.6 Tue 13:00 IFW B

Trajectory-based reconstruction in atom probe tomography — •Daniel Beinke, Christian Oberdorfer, and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

Atom probe tomography provides detailed three dimensional chemical information of a wide range of materials by the field evaporation of needle-shaped specimens. The field-evaporated ions are accelerated towards a detector and the time-of-flight as well as the hit position is measured. The reconstruction of the recorded detector events is critical in order to access the three dimensional information of the analyzed material. The standard reconstruction approach, introduced by Bas et al. [1], is based on a linear point projection between the measured detector position and a projection point located on the tip axis. The most remarkable success of this technique is the ability to recover lattice planes. However, characteristic artifacts occur, especially in the case of significantly different evaporation fields, i.e. near grain boundaries or in multicomponent layer structures. In this work, a concept for a reconstruction technique based on the calculation of realistic ion trajectories is presented. In a first step, the approach is tested on a rigid lattice [2]. Afterwards, the technique is expanded in order to deal with a limited detector efficiency and an unrestricted set of possible positions for the reconstruction of single atoms.

[1] P. Bas et al., Appl Surf Sci 87 (1995) 298-304. [2] D. Beinke et al., Ultramicroscopy 165 (2016) 34-41.

MM 33: Transport II - charge transport

Time: Tuesday 12:00–13:00 Location: IFW D

MM 33.1 Tue 12:00 IFW D

Combined resistivity and Hall effect study on Na(Fe,Rh)As single crystals — Frank Steckel[1], •Federico Caglieris[1], Robert Beck[1], Maria Roslova[2], Dirk Bombor[1], Igor Morozov[1,3], Sabine Wurmehl[1,4], Bernd Büchner[1,4,5], and Christian Hess[1,5] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany — [3]Department of Chemistry, Lomonosov Moscow State University, 119991 Moscow, Russia — [4]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [5]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

Electrical transport measurements are used to study the Rh-doped NaFeAs superconductor series with a focus on the tetragonal phase. The resistivity curvature has an anomalous temperature dependence evidencing in the phase diagram two crossover regions of changes in the scattering rate, the effective mass as well as of the charge carrier density. The first crossover region is directly connected to the structural transition and resembles the onset of resistivity anisotropy. The second crossover region can as well be deduced from the temperature dependent Hall coeffcient. A comparison to literature NMR data suggests this region to be connected with nematic fluctuations far above the tetragonal to orthorhombic phase transition.

MM 33.2 Tue 12:15 IFW D

Temperature dependence and lateral distribution of bias voltage driven charge transport through thin tantalum oxide films — •Jan Philipp Meyburg[1], Detlef Diesing[1], and Achim Walter Hassel[2] — [1]Institut für Physikalische Chemie, Universität Duisburg-Essen — [2]Johannes Kepler Universität Linz, 4040 Linz, Austria

The temperature dependence and the lateral distribution of currents in tantalum oxide (3–4 nm) based metal–insulator–metal devices induced by an applied voltage bias is studied from 80 K to 500 K. The sensitivity of the devices to a temperature change strongly depends on the polarity of the applied bias voltage. When the bias voltage weakens the internal field, the current increases by 4 orders of magnitude (Temperature increased from 400 K to 500 K). With bias voltages strengthening the internal field the current increases only by several 10 %. This asymmetry of the temperature dependence is strongly correlated with the asymmetry of the tunnel barrier and cannot be understood within the established Poole–Frenkel conduction or Schottky emission models. A new model presented here which fully includes the carrier transmission through a tilted barrier shows that tunnel emission explains the temperature dependences at different bias voltages.

MM 33.3 Tue 12:30 IFW D

Investigation of the conductivity-(micro-)structure correlation in Rectorite — •Wolfram Münchgesang[1], Anastasia Vyalikh[1], Juliane Weise[1], Maria T. Atanasova[2,3], Walter W. Focke[3], Gregor Mali[4], and Dirk C. Meyer[1] — [1]Technische Universität Bergakademie Freiberg, Institut für Experimentelle Physik, Freiberg, Germany — [2]Council for Geoscience, Pretoria, South Africa — [3]Institute of Applied Materials, Department of Chemical Engineering, University of Pretoria, Hatfield, South Africa — [4]National Institute of Chemistry, Ljubljana, Slovenia

The mixed-layer structure of Rectorite (Rt), made up of alternating nonexpandable (mica) and expandable (smectite) layers in a 1:1 ratio, can be used to transport and intercalate mobile ions like Na^+, Li^+, Sr^{2+} and Mg^+. Therefore Rt is in principle suitable as solid electrolyte and electrode in batteries. Starting from a crystallographic point of view, the changes of the temperature-depending complex conductivity of Rt with different by hydration replaced mobile species are discussed and correlated to structural and chemical data from solid-state nuclear magnetic resonance (NMR), powder diffractometry (PXRD) and X-ray photoelectron spectroscopy (XPS) measurements.
This work is financed by the Federal Ministry of Education and Research (BMBF) within the project SyNeSteSia (grant no 05K2014).

MM 33.4 Tue 12:45 IFW D

Platinum atomic contacts: from tunneling to contact — •Linda Angela Zotti and Ruben Perez — Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

We present a theoretical study of the electronic transport through Pt nanocontacts. We show that the analysis of the tunnelling regime requires a very careful treatment of the technical details. For instance, an insufficient size of the system can cause unphysical charge oscillations to arise along the transport direction; moreover, the use of an inappropriate basis set can deviate the distance dependence of the conductance from the expected exponential trend. While the conductance decay can be either corrected by employing ghost atoms or a large-cuto-radius basis set, the same does not apply to the corrugation, for which only the second option is recommended. Interestingly, these details were not found to have a remarkable impact in the contact regime. These findings are important for theoretical studies of distance-dependent phenomena in scanning-probe and breakjunction experiments.

MM 34: Poster session II

Time: Tuesday 18:30–20:30 Location: P4

MM 34.1 Tue 18:30 P4

The DFT (TB-mBJ) calculation of structural, electronic, elastic and vibrational properties of Mg2X(X=Si,Sn) — •MARFOUA Brahim[1], LIDJICI Hamza[1,3], and LAGHOUN Brahim[2] — [1]Laboratoire étude et développement des matériaux semi-conducteurs et diélectriques, Université de Laghouat, Route de Ghardaïa B.P.37G. Laghouat. Algérie. — [2]Laboratoire de physique des matériaux, Université de Laghouat, Route de Ghardaia B.P.73G. Laghouat. Algérie. — [3]Laboratoire des Matériaux et Procédés, Université de Valenciennes et du Hainaut-Cambrésis, Z.I du Champ de Abbesse 59600 Maubeuge, France

The semiconductors with the formula Mg2X (X= Si and Sn), have attract attention as potential high-performance thermoelectric materials, and their electonic, vibrational and thermal properties have extensively investigated [1-4]. They are an indirect band gap semiconductor [5-6]. We carried in this work an ab initio study based on the density functional theory to calculate structural, electronic, elastic and vibrational properties of Mg2X(X=Si and Sn). The FP-LAPW method was used with different form of exchange-correlation potential (LDA, GGA, PBEsol and mbj). TB-mBJ give the best result for the lattice parameter, and the best estimation of the band gap energy. Our results are in good agreement with experiment data available and other theoretical results.

MM 34.2 Tue 18:30 P4

Synthesis and analysis of electrodeposited Ni-P nanoglass — Farnaz Abdollahzadeh Davani, Stefan Ostendorp, •Martin

Peterlechner, Daniel Gaertner, Sergiy Divinskiy, and Gerhard Wilde — Institute of Materials Physics, Universität Münster, Münster, Germany

Nanoglasses, i.e. glassy materials characterized by two different nanoscaled glassy structures have recently been discovered. As yet, their structure, dynamics and stability are a matter of controversy. In the present work, electrodeposited amorphous Ni-P thin films with a granular sub-structure were chosen as a model system and layered granular structures were grown by applying pulsed voltages. Due to the relatively simple synthesis route and cheap costs the system is an excellent candidate for future studies on the nanoglasses. Using transmission electron microscopy and energy-dispersive X-ray spectroscopy it is shown that phosphorous-rich layers are fully amorphous. The glass transition was investigated by means of differential-and fast-scanning calorimetries. The bimodal structure and the broad glass transition signal are indications that the pulse-deposited Ni-P thin film is a nanoglass, according to the definition given in the literature. Thus, multilayerd nanocrystalline-nanoglassy systems can be prepared by pulsed electrodeposition and subsequent aging. The results are discussed with respect to the structure and stability of Ni-P nanoglass.

MM 34.3 Tue 18:30 P4

Nucleation Kinetics of deeply undercooled Germanium melts — •Manoel da Silva Pinto, Christian Simon, and Gerhard Wilde — Institut für Materialphysik - Wilhelm-Klemm Straße 10, 48149 Münster

In the classical nucleation theory the initial event of solidification is the stochastically formed metastable nuclei in the melt, which turn to be stable after exceeding the critical energy barrier. The statistical nature can be observed by the measurement of melting and solidification temperatures upon thermal cycling. By treating nucleation events as an inhomogeneous Poisson process, it is possible to estimate the nucleation rates from the undercooling values. Even an estimation of the interfacial energy applying classical nucleation theory is possible. The present work studies the nucleation of liquid germanium and estimates the nucleation rate and interface energy. We use differential thermal analysis to obtain sufficient big and accurate data sets. To avoid external nucleants and expel possible metal oxides from the sample, an inorganic glass is used as a fluxing agent and embedding medium.* A large undercooling is observed in pure germanium. The Gibbs free energy and the kinetic prefactor suggest a nucleation of heterogeneous nature. The geometric factor can be estimated and compared to the suggested value for this lattice system.

MM 34.4 Tue 18:30 P4

Friction under active control — •Victor Pfahl[1], Walter Arnold[2], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Universität Göttingen — [2]Department of Materials and Materials Technology, Saarland University

Dissipation of mechanical and kinetic energy at a sliding contact strongly depends on the topological structure and chemistry of the contact and on the dissipation mechanism of the underlying material. Instead of varying these mechanisms we are using external acoustic excitations and/or temperature variation to control friction actively.

Friction is measured with the lateral force microscopy (LFM) mode of an atomic force acoustic microscope (AFAM) and by studying microsliding in AFAM mode using acoustic excitation of the contact resonance frequency.

We investigated the reduction of friction of Si, amorphous PdCuSi and LaSrMnO as a function of amplitude of the cantilever at different temperatures. We can report a reduction of friction up to 100% on every system.

Due to a metal-metal transition near 350K temperature dependent measurements on LaSrMnO are interesting. The damping of the cantilever oscillations caused by micro-sliding of the cantilever tip on the surface decreases with temperature parallel to the increase in resistivity of the thin film. The behavior of the cantilever damping constant demonstrates that there is a direct coupling between mechanical friction and mobility of the electrons in the LSMO film.

We would like to thank the DFG for funding CRC 1073 Project A1.

MM 34.5 Tue 18:30 P4

Finite size corrections for periodic coupled cluster theory — Ke Liao[1] and •Andreas Grüneis[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department Chemie, Technische Universität München (TUM) Lichtenbergstrasse 4, D-85747 Garching, Germany

We present a method to correct for finite size errors in periodic coupled cluster theory calculations of solids. The newly developed method shares similarities with electronic structure factor interpolation methods used in quantum Monte Carlo calculations [1]. However, in the case of coupled cluster theory no explicit calculation of density matrices is needed [2]. We discuss the asymptotic behaviour of the correlation energy with respect to the total number of k-points used to sample the first Brillouin zone. Furthermore we present results showing that chemical accuracy in the convergence of coupled cluster correlation energies per atom can be achieved using two atomic unit cells and 3 x 3 x 3 k-point meshes only.

[1] M. Holzmann, R. C. Clay, M. A. Morales, N. M. Tubmann, D. M. Ceperley, and C. Pierleoni, Phys. Rev. B 94, 035126 (2016).

[2] K. Liao, and A. Grüneis, J. Chem. Phys. 145, 141102 (2016).

MM 34.6 Tue 18:30 P4

The Mg(111)/H$_2$O interface studied by empirical potentials and density functional theory using automated tools — •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

Modern supercomputers have made efficient electronic structure and atomistic simulation methods commonplace. Integrated computational materials design involves the combination of computational data associated with different length and/or time scales to aid materials discovery and the understanding of materials properties. However, the combination of different methods is often tedious in practice, since input and output of the employed methods have usually different formats. Our in-house python based computational materials library PyIron, handles this problem with the use of a database backend and the hierarchical HDF5 data storage format, which provides a user friendly interface to popular simulation packages. The capabilities of PyIron will be demonstrated using the Mg(111)/water interface, which is of interest for electrochemical applications. Water structures obtained by molecular dynamic simulations performed using an empirical TIP3P potential are easily integrated to provide a good starting configuration for the water structure used within the ab-initio calculations of the Mg(111)/H$_2$O interface. The then computed electronic structure provides insight into bonding and interactions at the metal water interface.

MM 34.7 Tue 18:30 P4

Spatially resolved in-situ defect spectroscopy with a positron beam during tensile tests — •Matthias Thalmayr, Thomas Gigl, Marcel Dickmann, Benjamin Rienäcker, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The positron beam facility NEPOMUC at the Research Neutron Source FRM II provides the worlds most intense mono-energetic positron beam with an intensity of 10^9 moderated positrons per second. The CDB spectrometer at NEPOMUC enables depth dependent and spatially resolved defect studies by using Doppler broadening spectroscopy (DBS), and measurements with coincident DBS. Among the numerous techniques applied for characterizing solids, (C)DBS is nondestructive and has an outstanding sensitivity on open volume defects like vacancies, dislocations and nano-voids. A novel device is presented that enables both, in-situ tensile tests and simultaneously spatially resolved high resolution defect spectroscopy of the specimen in the sample chamber of the upgraded CDB spectrometer. While recording the stress-strain curve of the specimen being deformed during conventional tensile tests, the changes of the lattice and in particular the formation of lattice defects and the increase of the defect concentration can be studied by analyzing the observables of the electron-positron annihilation process. With the new setup it will be possible to image the distribution of lattice defects at the annihilation site with an anticipated resolution in the micrometer range.

MM 34.8 Tue 18:30 P4

Comparing interatomic potentials for Si and Mo — •Yury Lysogorskiy, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Interatomic interaction potentials are widely used in computational materials science for simulations at the atomistic level. Nowadays a large number of interatomic potentials is available for a wide range of chemical elements and their mixtures [1,2]. We compare the most prominent interatomic potentials that are available for two prototypical elements, Si and Mo, with respect to predictions from density functional theory calculations. The comparison of the potentials is done at two levels. First, a number of properties of the potentials are evaluated. This includes the cohesive energy, atomic volume, elastic coefficients, vibrational properties, thermodynamic potentials, and defect formation energies for relevant crystal structures. From this a fingerprint characterisitic of the performance of the potential is derived. Second, the data is used to qualify a given potential for situations that were not explicitly tested at the first step, i.e. to assess the transferabilty and predictive capability of a potential. We illustrate the very different behaviour of the potentials and relate this to the functional form of the potential as well as the purpose for which the potential was originally fitted.

[1] E. B. Tadmor, R. S. Elliott, J. P. Sethna et al. Knowledgebase of Interatomic Models (KIM). https://openkim.org, 2011

[2] C.A. Becker, et al. Curr. Opin. Solid State Mater. Sci., 17, 277-283 (2013).http://www.ctcms.nist.gov/potentials

MM 34.9 Tue 18:30 P4

Ab initio study of planar defects in Ni and Co based superalloys — •Aparna P. A. Subramanyam, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr University-Bochum, Bochum, Germany

Single-crystal Ni-based and Co-based superalloys are used in high temperature applications in land-based turbines and jet engines. These alloys exhibit resistance to deformation at high temperatures due to precipitates of $L1_2$-Ni_3Al type. One important deformation mechanism of plastic deformation is dislocation shearing of the precipitates by the formation of planar defects.

In this study, we investigate the structural stability of superlattice intrinsic and extrinsic stacking faults (SISF, SESF), anti-phase boundaries and complex stacking faults in the $L1_2$ phase of Ni_3Al and $(Co/Ni)_3Al$ using density functional theory calculations. The segregation of alloying elements to the stacking faults is analysed for the technologically important alloying elements Re, W and Cr. These results are compared to the segregation to twin boundaries in Ni_3Al and $Co_3(Al/W)$.

MM 34.10 Tue 18:30 P4

Effect of Al alloying on the martensitic temperature in Ti-Ta shape memory alloys — •Alberto Ferrari, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44780 Bochum, Germany

Ti-Ta-based alloys are promising candidates as high temperature shape memory alloys (HTSMAs) for actuators and superelastic applications. The shape memory mechanism involves a martensitic transformation between the low-temperature α'' phase (orthorhombic) and the high-temperature β phase (body-centered cubic). In order to prevent the degradation of the shape memory effect, Ti-Ta needs to be alloyed with further elements. However, this often reduces the martensitic temperature M_s, which is usually strongly composition dependent. The aim of this work is to analyze how the addition of a third element to Ti-Ta alloys affects M_s by means of electronic structure calculations. In particular, it will be investigated how alloying Al to Ti-Ta alters the relative stability of the α'' and β phases. This understanding will help to identify new alloy compositions featuring both a stable shape memory effect and elevated transformation temperatures.

MM 34.11 Tue 18:30 P4

Deformation Mechanisms in Magnetron Sputtered Thin Film Metallic Glasses — •Marlene Mühlbacher[1], Christoph Gammer[2], Ruth Konetschnik[1], Thomas Schöberl[2], Christian Mitterer[1], and Jürgen Eckert[1,2] — [1]Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Erich Schmid Institute for Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, 8700 Leoben, Austria

Amorphous metallic coatings have recently emerged as promising thin film materials due to their excellent chemical stability, good wear resistance and exceptionally high strength. Their mechanical behavior, however, is fundamentally different from their crystalline counterparts, due to the disordered structure lacking dislocations as carriers of plastic deformation. To investigate the different deformation mechanisms, we have synthesized Pd-based crystalline/amorphous multilayer systems by unbalanced dc magnetron sputtering. Hardness and Young's modulus of the multilayer systems are assessed by nanoindentation. Indents are evaluated by atomic force microscopy and scanning electron microscopy for a quick estimation of the coatings' response to plastic deformation. Micromechanical samples of selected systems are prepared in a focused ion beam instrument. Deformation mechanisms and their dependence on layer arrangement are then investigated with a particular emphasis on in-situ tensile testing and bending in the electron microscope. This approach allows for a direct comparison of plastic deformation through the movement of dislocations and shear bands in the crystalline and glassy layers, respectively.

MM 34.12 Tue 18:30 P4

Ab initio investigation of Re-Re interactions in Ni-base superalloys — •Maximilian Grabowski, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Deutschland

Ni-base superalloys are widely used in high-temperature applications e.g. in turbine blades for jet engines of aeroplanes. In these applications, the materials have to perform at high temperature and high stress. Ni-base superalloys have a complex composition where one of the key ingredients is Re, which significantly improves the mechanical behaviour.

Using density functional theory (DFT) calculations we investigate the Re-Re interaction in Ni with a particular focus on the role of magnetism. The nearest neighbour Re-Re interaction in the nonmagnetic and in the ferromagnetic configuration exhibit a qualitatively different behaviour from strongly repulsive to weakly attractive. We show that this is mainly due to a decrease of the Ni magnetic moment in the vicinity of Re and discuss possible consquences for the clustering of Re in Ni-based superalloys. In a next step we investigate the mobility of Re in Ni in concentrated Ni-Re alloys. As a basis for our dynamical simulations, we use a cluster expansion (CE) to evaluate the energies of the binary Ni-Re and the ternary Ni-Re-Vacancy system. DFT calculations are used to determine the effective cluster interactions (ECI) for the CE. We will also report on our progress of a CE for the diffusion barriers, which -when converged- enables us to predict diffusion in concentrated Ni-Re alloys from first-principles calculations.

MM 34.13 Tue 18:30 P4

Implementation of nonlocal van der Waals functionals into the LAPW method — •Fabien Tran, Julia Stelzl, and Peter Blaha — Vienna University of Technology, Institute of Materials Chemistry, A-1060 Vienna, Austria

The so-called van der Waals density functionals (vdW-DF) [1], which are much more reliable than the traditional semilocal functionals for systems where the dispersion forces play a major role, are nonlocal in the sense that they consist of a double integration over the space. Therefore, the implementation of vdW-DF is much more involved and the computational time is higher compared to semilocal functionals. For plane-wave pseudopotential methods, an efficient algorithm proposed by Román-Pérez and Soler [2] based on fast Fourier transform was proposed, such that the vdW-DF are nowadays widely used in the pseudopotential community. However, for all-electron densities, the scheme of Román-Pérez and Soler can not be applied efficiently, since a plane-wave expansion of the all-electron density would require an extremely huge number of terms. In this work, a smoothing procedure of the all-electron density in a region around the nucleus is applied, such that the scheme of Román-Pérez and Soler can be applied efficiently. This is done in the framework of the all-electron linearized augmented plane-wave (LAPW) basis set as embodied in the WIEN2k code. The obtained results are compared with results from the literature.

[1] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).

[2] G. Román-Pérez and J. M. Soler, Phys. Rev. Lett. **103**, 096102 (2009).

MM 34.14 Tue 18:30 P4

Impact of magnetism on the stability of Laves phases in Fe-Nb alloys — •Ali Zendegani[1], Alvin N. Ladines[2], Thomas Hammerschmidt[2], Ralf Drautz[2], Fritz Körmann[1], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

Ferritic steels containing Fe-Nb Laves phases have a number of industrially relevant high-temperature applications, e.g., for automotive industry. The Laves phases play a decisive role for the high-temperature strength of these materials. To tailor their mechanical characteristics, e.g., via heat treatments, a precise knowledge of the Laves phase thermodynamic stability is essential.

We have investigated the phase stability of the three different Laves phases in Fe-Nb alloys, i.e. hexagonal C14 and C36, and cubic C15, combining density functional theory and thermodynamic concepts. The ground state energy as well as finite temperature entropy contributions of these structures are evaluated for various magnetic configurations, ranging from non-magnetic simulations over selected ferro/ferrimagnetic ones to fully paramagnetic calculations. We discuss the challenges and methodological advances developed for such computations.

MM 34.15 Tue 18:30 P4

Properties of mechanically intermixed Cu-Ta alloys — •Regina Post, Nazar Ibrahim, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Copper and tantalum are known to be fully immiscible and do not form an alloy by cooling from the liquid state. They can however be forced to mix by severe plastic deformation methods, such as high pressure torsion (HPT). Using HPT on a stack of alternating Cu and Ta thin foils, different mixing states can be created.

The present study is focused on the evolution of the microstructure with increasing number of revolutions of the HPT process by comparison of the cross section and plain view structures via orientation imaging microscopy applying the EBSD analysis. The microstructure of copper-rich grains is found to be remarkably stable even after annealing at high temperatures of about 95% of the copper melting point. The appearance of the Cu-Ta solid solution is investigated by TEM analyses and the results are discussed in terms of the mixing mechanism.

MM 34.16 Tue 18:30 P4

Quantitative High-resolution TEM Imaging of Perovskite Interfaces — •Tobias Meyer[1], Patrick Peretzki[1], Benedikt Ifland[2], Birte Kressdorf[2], Christian Jooss[2], and Michael Seibt[1] — [1]IV. Physical Institute, University of Göttingen, Germany — [2]Institute for Materials Science, University of Göttingen, Germany

The Shockley-Queisser limit for single junction solar cell efficiencies is based on energy losses due to the transmission of low energy photons with energies below the band gap and the thermalization of hot charge carriers. In strongly correlated perovskite materials, which exhibit polaronic charge carriers, these losses can be reduced at the same time by harvesting long-living intraband excitations. Indeed, during the last decade the efficiency of halide perovskite based solar cells has been increased from 2 % to 20 %. However, the underlying materials are relatively instable – particularly under light illumination. In contrast to halide perovskites, transition-metal oxides are rather stable but their junctions exhibit lower photovoltaic energy conversion efficiencies. Since the electrical transport properties of these materials are highly dependent on the structure, a thorough understanding of the latter close to the interface is exceedingly desirable in order to tune perovskite junctions for photovoltaic applications. We investigated the structure of transition-metal oxide heterojunctions, i.e. the oxygen positions, in an image corrected high-resolution TEM. In order to enhance the contrast of the light oxygen columns, we used optimized conditions for the spherical aberration.

MM 34.17 Tue 18:30 P4

In-situ Electron Microscopy Studies of Electric Field Assisted Sintering of Oxide Ceramics — •Danny Schwarzbach, Max Steinbrück, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

A wide range of studies show a dramatic effect of applied electric fields or currents on the sintering behavior of oxide ceramic powders. However, the mechanisms accounting for these strong effects remain elusive despite the wide application potential.

By using in-situ scanning and transmission electron microscopy, material changes during sintering of model oxide ceramics (e.g. ZnO) will be directly observed. The evolution of microstructure and morphology, including grain/void morphology, segregation, and precipitation, will be tracked, both with and without applied fields and currents. The results will be compared to models to determine the dominant driving forces and mechanisms for sintering, and how these are affected by fields and currents. In addition, in-situ high resolution and electron holography studies, EELS, and in-situ studies under oxidizing and reducing atmospheres will be used to gain insight into the atomic origins of sintering behavior, as well as of high conductivity states that occur in conjunction with flash events during field-assisted sintering.

Due to the fact that this project has just started, the focus of this poster is to present the above-mentioned methods and to provide an overview of the current state of research. Nevertheless, some initial results are already expected.

Support of SPP 1959 by the DFG is gratefully acknowledged.

MM 34.18 Tue 18:30 P4

Mechanical Analysis of Metallic Glasses in the Non-Linear Regime — •Clemens Garve, Birte Riechers, and Konrad Samwer — Georg-August-Universität Göttingen

Amorphous metals are used in various applications, however the strongly temperature dependent viscoelastic behavior under deformation is not fully explained yet. To gain more understanding we deform a Palladium-based metallic glass using oscillatory stresses with amplitudes sufficiently high to drive the system beyond the Hookian regime of linear response.

Following experimental approaches used in dielectric spectroscopy [1] an oscillating mechanical stress was applied, which was switched from a low to high stress amplitude and back using a dynamical mechanical analyzer. By using Fourier analysis, we were able to separate our data into nonlinear contributions at fundamental and higher harmonic frequencies. While deforming with high stresses and in the following low stress section, the nonlinear contributions show time-dependent behavior, which was characterized to extract the time-scale of structural recovery [2]. The temperature and stress dependence of nonlinear contributions regarding amplitude and timescale were investigated.

We acknowledge support by DFG Research Unit FOR1394.

Citations: [1] Huang and Richert. "Dynamics of glass-forming liquids..." J. Phys. Chem. 124.16 (2006) [2] Riechers, Samwer, and Richert. "Structural recovery in plastic crystals by time-resolved nonlinear dielectric spectroscopy." J. Phys. Chem. 142.15 (2015)

MM 34.19 Tue 18:30 P4

system identification for nanodevices based on anodic alumina oxide (AAO) templates — •Jesus Alan Calderon Chavarri[1], Min Zhou[2], and Yong Lei[3] — [1]TU Ilmenau, Ilmenau, Germany — [2]TU Ilmenau, Ilmenau, Germany — [3]TU Ilmenau, Ilmenau, Germany

Nanodevices based on AAO templates (like nanotubes, nanorods, and nanowires) have interesting properties which can be described by a mathematical analysis in order to propose mathematical modelings based on linear behavior. In this scenery, it can be demonstrated mathematically, some of their characteristics which are controllability and stabillity. Therefore, as it is shown in this work, it is proposed correlations among characteristics of nanodevices based on AAO templates with mathematical operations to identify physical properties of them through linear range of work. Furthermore, it can be tested different System Identification methodologies in order to get physical parameters, or to identify response of these nanodevices in front of input excitation signals. As a consequence, it is possible to design different algorithms to get optimization and predictions of physical properties, because of this system identification based on correlations proposed.

MM 34.20 Tue 18:30 P4

Mechanically tuned stress state of palladium thin films on rutile titanium dioxide — •Maximilian Litschauer[1], Marian David Bongers[1], Daniel Harding[2], Alec Wodtke[2], and Astrid Pundt[1] — [1]Institut für Materialphysik, Univ. Göttingen — [2]Institut für Physikalische Chemie, Univ. Göttingen

The mechanical stress state of epitaxially grown palladium (Pd) thin films on Al_2O_3 single crystals can be varied by the film thickness [1]. This stress state may also affect the surface conditions, for example by modifying the distance between the Pd surface atoms. This should result in a modified surface reactivity as suggested for example by the d-band model of Mavrikakis et al. [2]. In this study the stress states of differently prepared Pd films on titanium dioxide (TiO_2) is presented and the binding energies (BE) of carbon monoxide (CO) on these surfaces is determined. Therefore, the deposition temperature and film thickness of Pd thin films are varied. The films are deposited by magnetron sputtering on pretreated $TiO_2(110)$ substrates. The stress state is characterized by X-ray diffraction via the Pd(111) peak shift. The related BE are addressed by using a novel ion imaging technique to directly measure the microsecond lifetime of CO on the surface [3]. The results are discussed with respect to the mechanical stress states.

This study is supported by the Deutsche Forschungsgemeinschaft via SFB1073, project C06 and C04 as well via the Heisenberg grant PU131/9-2. [1] S. Wagner et al., Acta Materialia 114 (2016) 116; [2] M. Mavrikakiset al., Phys. Rev. Lett. 81 (1998) 2819; [3] D. J. Harding et al., J. Phys. Chem. A 119 (2015) 12255

MM 34.21 Tue 18:30 P4

AiiDA Workflows with FLEUR for X-ray Photoelectron Spectroscopy — •Jens Bröder[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Rudi Koslowski[2], Christian Linsmeier[2], and Stefan Blügel[1] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We present the plug-in of the all-electron DFT code FLEUR [1] to AiiDA [2] (Automated interactive Infrastructure and database for material science) and our first established workflows to calculate electron binding energies and core level shifts (CLS) of X-ray photoelectron spectroscopy (XPS) of pure materials for surface science.
One workflow calculates CLS in the initial state approximation of bulk and slab geometries. Another workflow uses super cell core-hole calculations to extract binding energies. Their first application will be on materials relevant for research on plasma wall interaction in fusion. First results of different methods are compared to recent experimental data.

We acknowledge partial support from the EU Centre of Excellence "MaX Materials Design at the Exascale" (Grant No. 676598).

[1] www.flapw.de
[2] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)

MM 34.22 Tue 18:30 P4

Lateral H-Diffusion in Mg thin films — •Niklas Teichmann, Magnus Hamm, and Astrid Pundt — Univ. Göttingen, IMP, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Hydrogen in metals like Magnesium changes the physical properties of the host material, such as the optical properties.[1] The optical light transmission can be used to determine locally the Hydrogen content, or to differentiate between phases (Hydrogenography).[2] For the Mg-H system, two phases are relevant at 300 K: the metallic α-phase and the transparent MgH_2-phase.
In this presentation, the hydrogen-induced optical change of thin Mg-films is investigated using electrochemical loading via a Pd-gate.[3] By this, the lateral diffusion and the MgH_2 formation can be directly seen and the formation kinetics can be studied. The influence of grain boundaries is discussed.
Financial support by the DFG via projects PU131/9-2 and PU131/10-2 is gratefully acknowledged.
[1] T. Richardson et al. Applied Physics Letters 78.20 (2001): 3047-3049.
[2] R. Gremaud et al. Advanced Materials 19.19 (2007): 2813-2817.
[3] J. Kürschner et al. Journal of Alloys and Compounds 593 (2014): 87-92.

MM 34.23 Tue 18:30 P4

Computional study of Y NMR shielding in intermetallic yttrium compounds — •Leila Kalantari and Peter Blaha — Institute of Material Chemistry, Vienna University of Technology, Getreidemarke 9/165-TC, A-1060 Vienna, Austra

Density functional theory calculations of the magnetic shielding for solid state nuclear magnetic resonance (NMR) provide an important contribution for the understanding of the experimentally observed signals. In this work, we present calculation of the Y NMR shielding in intermetallic compounds. (YM, YMX, YM_2X, YM_2X_2, Y_2MB_6 and Y_2MSi_3 where M represents various transition metals and X refers to Si, Ge, Sn). The total shift σ of this selection varies by about 2500 ppm and correlates very well with the experimentally observed shielding except for YMg and YZn. These two simple compounds have a spike in the DOS at E_F and a corresponding huge spin susceptibility which lead to the disagreement. The diamagnetic contribution σ_o (chemical shift) is by no means constant as often assumed when interpreting experimental metallic shifts and varies up to 1700 ppm, but still the dominating term is the spin contact term σ_c. Although all compounds are metals, only half of them have a paramagnetic (negative) σ_c due to reoccupation of the valence Y-5s electrons, while for others the induced Y-4d magnetic moment induces diamagnetic core contributions. In all our cases the spin dipolar contribution σ_{sd} is fairly small and $|\sigma_{sd}|$ is less than 200 ppm and often even much smaller except in a few very asymmetric compounds like Y_2ReB_6 ($\sigma_{sd} \approx 450 ppm$)

MM 34.24 Tue 18:30 P4

AUXILIARY-MODE APPROACH TO TIME-DEPENDENT PHONON TRANSPORT — •Leonardo Medrano Sandonas[1,2], Alexander Croy[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,3,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany. — [3]Dresden Center for Computational Materials Science, Dresden, Germany. — [4]Center for Advancing Electronics Dresden, Dresden, Germany.

Next to electrons, phonons play a major role for the behavior of nanoscale devices. Additionally, phononics and nano-mechanics offer the possibility to steer and manipulate phonons. Hence, a more detailed understanding of phonon dynamics is required. Using an auxiliary-mode approach, which has successfully been applied for the case of electrons, we present a method to describe time-dependent phonon transport based on the time-dependent Green's function formalism. This allows us to study local vibrations which are driven by time-dependent temperature differences between heat reservoirs.

MM 34.25 Tue 18:30 P4

Effects of surface diffusion and surface roughness on plastic behavior of nanoporous gold — •Jie Li[1], Nadiia Mameka[1], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, Hamburg, Germany

The microstructure of dealloying-derived nanoporous metals may be understood as a network of interconnected single nanowires (or nanoligaments). The availability of millimeter-size samples of these nanomaterials predestine them for fundamental studies of small-scale effects on the mechanical behavior. While recent experiments and simulations have acknowledged important effects of ligament size along with solid fraction and network connectivity on both elastic and plastic deformation, the role of surface effects and their precise origin remain to be clarified. Among relevant microscopic processes at the surface are impact of the *surface diffusion* and *atomic-scale surface roughness* on the plastic behavior of the high surface area materials are explored in this study. We probe the plastic response of nanoporous gold to changes of the surface diffusion constant and surface roughness or smoothness of the nanoligaments by deforming the material in situ in an electrochemical cell with various surface conditions. The relationships between different surface morphologies induced in our experiments by the exposure to the specific electrochemical environments and the plastic behavior are discussed.

MM 34.26 Tue 18:30 P4

Grain refinement in ball-milled nanocrystalline iron-boron — •Max Steinbrück — IMP Universität Göttingen

In this thesis, iron-boron alloys were produced and the influence of the concentration of boron on the grain size was investigated. In theory, the relatively small boron atoms should segregate to the grain boundaries of iron. This reduces the surface energy of the grains and therefore favors the formation of grain boundaries and reduces grain growth. To investigate this, Fe and FeB powder were ball-milled to produce alloys with different boron concentrations. The grain size was determined by transmission electron microscopy and x-ray diffraction. It could be shown that in the investigated interval up to 17,3 at.% the grain size decreases with increasing boron concentration. The thermal stability of the powder was examined by differential scanning calorimetry, where a phase transition while heating and the formation of a Fe2B phase were observed. The results were connected to previous works on iron-oxygen and iron-carbon systems.

MM 34.27 Tue 18:30 P4

Mechanical stress upon hydrogen absorption in Nb-Fe Films — •Philipp Klose, Magnus Hamm, and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Hydrogen absorption in thin films adhered to rigid substrates results in compressive mechanical in-plane stresses.[1,2,3] These stresses can lead to changes in the material*s properties. While the in-plane film stress increases linearly on the hydrogen content for low hydrogen concentrations, deviations from the linearity appear at the yield stress [3,4]. The yield stress inversely depends on the film thickness.[5] For hydrogen loaded Niobium films, linearity is maintained to 1 H/Nb, for films below 7 nm and mechanical stress of up to -10 GPa is achieved.[5]

The yield stress can also be affected by alloying. In this presenation we study the stress-development upon hydrogen loading in niobium-iron (about Nb90-Fe10) films. Films of different thickness were prepared by argon-cathode beam sputtering. Hydrogen loading was performed from the electrolyte using constant current conditions. For these films, stress linearity is found up to at least 40 nm film thickness.

This work is financially supported by the DFG via project PU131/12-1. [1] J. Weissmuller and C. Lemier, Philos. Mag. Lett. 80:6 (2000), [2] S. Wagner and A. Pundt, Appl. Phys. Lett. 92.5 (2008), [3] U. Laudahn et al., JALCOM 1999 ,[4] A. Pundt, et al., Phys. Rev. B 61.15 (2000), [5] Hamm, M., et al. "Achieving reversibility of ultra-high mechanical stress by hydrogen loading of thin films." Applied Physics Letters 106.24 (2015): 243108.

MM 34.28 Tue 18:30 P4

Tuning the amorphous phase of the Phase change materials GeSbTe225 and Sb2Te by altering the quenching-rate from the liquid phase — •Christoph Persch, Thorben Frahm, and Matthias Wuttig — 1.Physikalisches Institut IA, RWTH Aachen University, 52074 Aachen, Germany

Phase-change materials (PCMs) constitute a class of materials characterized by a pronounced difference in physical properties between the crystalline and the amorphous phase. The crystalline state usually features a low electric resistance and a high reflectivity while the amorphous state features a high electric resistance and a low reflectivity. As phase transitions are inherently fast, phase-change materials are of great interest for non-volatile memory applications, such as solid state PC-RAM. To investigate the switching behavior of phase-change materials, a measurement setup comprised of a pulse-probe laser system and a detection unit has been established. To deposit a sufficient amount of thermal energy in the PCM sample under investigation, the PCM layer is situated in a layer stack constituted of dielectric materials. This allows for a fine tuning of the heat flow into the substrate material upon heating and upon melt-quenching, so by altering the thickness of the dielectric layers, different quenching rates (q.r.) could be obtained. A significant change of the temperature-dependent crystal growth velocities in the amorphous phase of PCMs quenched at different rates has been observed. Thus, tuning the amorphous phase of PCMs by altering the q.r. has been demonstrated, rendering the q.r. another important factor to consider in the process of device-design.

MM 34.29 Tue 18:30 P4

Computational thermodynamics applied to battery materials — •Sebastian Schwalbe[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Technische Universität Dresden, Theoretical Chemistry, Germany

From the computational point of view battery materials (e.g. Li_xSi_y, Li_xSn_y or $FePO_4$) are numerically very demanding, as they are described by large unit cells with up to hundreds of atoms. We present ab-initio thermodynamic data sets (e.g. isobaric heat capacities) calculated in the framework of density functional theory and the quasi-harmonic approximation. Further, we used force-field potentials to reproduce ab-initio thermodynamic data reducing computational time [1]. Our goal is the construction of the phase diagram based on calculation without the need of experimental input.

[1] Schwalbe et al., arXiv preprint arXiv:1610.08991

MM 34.30 Tue 18:30 P4

Hydrogen Diffusion in Magnesium: Influence of Grain Boundaries — •Felix Jung[1], Magnus Hamm[1], Jakub Cižek[2], and Astrid Pundt[1] — [1]Institute for Material Physics, Georg-August-Universität Göttingen, Germany — [2]Department of Low-Temperature Physics, Charles University, Prague, Czech Republic

Grain boundary (GB) diffusion differs from bulk diffusion in crystals. For substitutional solvents in metals, GB diffusion is several orders of magnitude faster, for interstitial solvents it can be either slower or faster, depending on the solvent concentration [1,2]. In this work the diffusion of hydrogen gas in the magnesium-hydrogen system is used as a model system. To explore the dependence of the diffusion coefficient on grain boundaries, the sample grain size is varied, thereby achieving differing grain boundary volume fractions. Additionally, the difference between the metallic magnesium and the hydride phase is studied. Magnesium thin films and ECAP treated bulk magnesium samples are characterized using optical and electron microscopy. Purity and grain structure of the bulk samples are investigated by EDX and EBSD measurements. Hydrogen gas volumetry is used to determine the diffusion behaviour in the α-regime and the hydride phase and to calculate the related diffusion coefficients. Financial support provided by the Deutsche Forschungsgemeinschaft via the projects PU131/9-2 and PU131/10-1 is gratefully acknowledged. [1]I. Kaur und W. Gust, Fundamentals of grain and interphase boundary diffusion, Stuttgart: Ziegler Press, (1989) [2]T. Muetschele and R. Kirchheim, Scripta Metallurgica 21, 135-140 and 1101-1104, (1987)

MM 34.31 Tue 18:30 P4

Polypyrrole confined in porous silicon: From fundamentals to applications — •Manuel Brinker[1], Guido Dittrich[1], Philipp Timm[1], Thomas Keller[2,3], Pirmin Lakner[2], and Patrick Huber[1] — [1]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg (TUHH), Eißendorfer Straße 42, 21073 Hamburg — [2]DESY NanoLab FS-NL, Research Group X-ray Physics and Nanoscience, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg — [3]Departement Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

We investigate the properties of the semi-conducting polymer polypyrrol (PPy) in parallel, tubular pores of monolithic micro- (pore diameter $D < 2nm$)-, meso- ($2 < D < 20nm$) and macroporous ($D > 50$ nm) silicon (PSi). On the one hand PPy offers the opportunity to modify the electrical conductivity of the PSi, while sensoric and actoric applications for the PPy/PSi hybrid system are possible as well. We investigate the electrochemical polymerisation process of PPy in PSi [1] with regards to the orientation of the molecules in the pores and the role of the pore surfaces. [1] F.A.Harraz, Electrochemical formation of a novel porous silicon/polypyrrole hybrid structure with enhanced electrical and optical characteristics, J. Electroanal. Chem. 729 (2014) 68*74.

MM 34.32 Tue 18:30 P4

Potential-strain coupling on electrocatalysis of nanoporous platinum — •Xinyan Wu[1], Shan Shi[1,2], Anastasia Strasser[1], Matthias Graf[1], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg — [2]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht

Nanoporous platinum derived from dealloying shows excellent electrocatalytic activity such as methanol electrooxidation due to their extremely high specific surface area. Elastic deformation is known to strongly impact many chemical reaction processes. So it is of great interest to detect and quantify the coupling of catalysis reaction to strain in nanoporous platinum. Here we fabricated nanoporous platinum thin films by dealloying cosputtered Pt-based alloys. Then we explored the influences of elastic strain on the methanol electrooxidation process (reaction potential, rate and efficiency, etc.) via dynamic electro-chemo-mechanical analysis (DECMA).

MM 34.33 Tue 18:30 P4

in-situ TEM observations of motions of nanostructures entrapped in carbon nanotube — kecheng cao[1], johannes biskupek[1], thilo zoberbier[1], thomas w. chamberlain[2], andrei n. khlobystov[2], and •ute kaiser[1] — [1]Central Facility for Electron Microscopy, Ulm University, Ulm, Germany — [2]School of Chemistry, University of Nottingham, Nottingham, UK

Single-walled carbon nanotubes (SWNTs) are promising materials to realize the controllable transport of molecules due to their narrow cylindrical cavities. Time-resolved in-situ transmission electron microscopy (TEM) imaging with an atomic resolution enables direct visualization of molecular motion in SWNTs. The back and forth translations of a carbon capsule, LaC2 nanocrystal, C60 molecules in SWNTs have been subsequently reported. However, the driving mechanism of these motions is still unknown.

In this study we follow translational motion of different types of nanoparticles investigated by means of 30 and 80 kV time-resolved in-situ TEM in order to deduce the driving force of the motion. Prior to electron beam irradiation, the SWNTs were filled with Fe3(CO)12 molecules, which then converted into α-Fe nanoparticles and Fe compounds with amorphous carbon in the lumen of SWNTs.The reciprocating motions of Fe nanoparticles were observed and recorded. We demonstrated the electrostatic repulsion due to ionization of the nanoparticles by the electron beam as the most likely force propelling the nanoparticles in their translational motion.

MM 34.34 Tue 18:30 P4

Imaging and kinetics of MgH2 and TiH2 formation — •Efi Hadjixenophontos[1], Lukas Michalek[1], Manuel Roussel[1], Andreas Weigel[1], Toyoto Sato[2], Shin-ichi Orimo[2,3], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft, (IMW) University of Stuttgart, Heisenbergastrasse 3, 70569 Stuttgart, GERMANY — [2]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 JAPAN — [3]WPI-Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 JAPAN

Among the metal hydrides, Mg and its alloys show an excellent performance for the H-fuel based economy.In order to improve the system, it is first important,to understand the reason for the slow kinetics of hydride formation, which is surprisingly still an open field of research and the focus of this work. TM-metals,have shown to lower the activation energy, and therefore improve the kinetics.Here we study separately the two systems: MgH2 with Pd as catalyst, and TiH2 thin films and compare them to their bulk behaviour.The two metals show a different mechanism of hydrogenation, and the oxide layer in the case of Ti seems to have a great impact. Hydrogen diffuses in Ti faster and TiH2 is first formed closer to the substrate.In the case of Mg a microscopic imaging of the co-existence of the hydride and pure phases shows that MgH2 is immediately formed at the interface between the Pd catalyst coating and the Mg thin film and it grows in a layer-like reaction towards the substrate.XRD,SEM-FIB and TEM are the combined techniques used to discus the diffusion coefficients and mechanisms of hydrogenation.

MM 34.35 Tue 18:30 P4

Single-spin hybridization expansion continuous-time Monte Carlo for time-dependent Anderson impurity model — •Patryk Kubiczek[1], Alexey Rubtsov[2], and Alexander Lichtenstein[1] — [1]Institute of Theoretical Physics, University of Hamburg, Germany — [2]Russian Quantum Center, Moscov, Russia

In this work we propose a modified version of the standard continuous-time hybridization expansion quantum Monte Carlo method (CT-HYB-QMC) in which the expansion is performed only for a single-spin channel. At the same time the effective single-particle Schrödinger equation for the other spin-channel is solved explicitly. We apply this method to the time-dependent Anderson impurity model and show that it leads to the sign problem alleviation, which makes it possible to find the exact solutions of the model for larger timescales.

MM 34.36 Tue 18:30 P4

Diffusion in intermetallic $AlAu_4$: MD study down to temperatures relevant to wire bonding — •Mohammed Guerdane — Karlsruhe Institute of Technology, IAM-CMS, Karlsruhe

We show the ability of long time ($\sim 1\mu s$) molecular dynamics modeling to provide quantitative diffusion coefficients for the compound $AlAu_4$ (β-Mn type), down to temperatures ($\sim$ 200 °C) that are relevant to Al-Au wire bonding. Concerning Au diffusion, our results agree quite well with DFT calculations of the vacancy-formation energy, the activation energy, and the diffusion mechanisms. The van Hove correlation-function analysis shows that Au diffusion takes place mainly on the Wyckoff **b** sublattice. Moreover, we shed light on the high-temperature region, as the stability limit $T^\star$ of $AlAu_4$ is approached and unfavorable jumps contribute to the diffusivity. This concerns, for instance, jumps generating antisites defects. The latter lead to a massive disorder which ends up in a phase change to a distorted fcc structure at $T^\star$. Including the melting temperature in the potential-fitting procedure seems to be an effective way to gauge the temperature scale and properly capture the order of magnitude of diffusion.

MM 34.37 Tue 18:30 P4

Thermal Diffusivity Measurements with Single Particle Photothermal Microscopy — •André Heber and Frank Cichos — Universität Leipzig, Exp. Phys. I, Molecular Nano-Photonics Group, Leipzig, Germany

Photothermal single particle microscopy has proven to be a sensitive imaging technique for absorbing nanoparticles and molecules. Here, we discuss the extension of photothermal microscopy to the measurement of thermal diffusivities in the surroundings of an absorber. The photothermal contrast makes use of a heating induced refractive index change. As the refractive index change is small a modulated heating scheme is implemented in which the optical heating is harmonically modulated and the detection laser detects fluctuations at that particular modulation frequency. This configuration enables a high signal to noise ratio and adds a time scale for the measurement of thermal transport as the temperature profile is not instantly established. Here, we show how single particle microscopy can be used to sense anisotropies in the thermal transport and interfaces using single particle photothermal microscopy.

MM 34.38 Tue 18:30 P4

Electron transport in nanoparticle networks — •Michael Deffner[1], Florian Schulz[2], Carmen Herrmann[1], and Holger Lange[2] — [1]Institut für Anorganische und Angewandte Chemie, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Deutschland — [2]Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117 20146 Hamburg, Deutschland

Gold nanoparticles (AuNPs) are a stable and easy-to-functionalize platform for different purposes such as medical imaging or sensor applications. AuNPs can be functionalized by straightforward ligand exchange for example with thiols or amines, which bond easily to the surface of the nanoparticle and can induce aggregation processes.

In order to systematically study the transport properties of gold nanoparticle clusters, in a first step the formation of networks and clusters of AuNPs are studied using biphenyl-4,4'-dithiol, p-terphenyl-4,4"-dithiol and 1,9-nonane-dithiol as molecular linkers.

Electron transport properties of these networks are studied using terahertz spectroscopy as well as transport calculations for single gold–molecule–gold junctions following the Landauer–Büttiker formalism. Within this approach, electron transport is described as a tunneling problem which can be solved using quantum chemical software.

MM 34.39 Tue 18:30 P4

Effect of surface reconstruction on the exchange interactions in CaMnO3 — •Samara Keshavarz — Uppsala University, Uppsala, Sweden

The effects of geometrical relaxation at the surface as well as the change of crystal field are mostly able to influence the lower energy magnetic configuration. In particular, our analysis of CaMnO3 surface reveals that the exchange interaction between the Mn atoms belonging to the surface and the subsurface layers is very sensitive to the structural changes. An earlier study [A. Filippetti and W.E. Pickett, Phys. Rev. Lett. 83, 4184 (1999)] suggested that this coupling is ferromagnetic and gives rise to the spin flip process on the surface of CMO. In our work we confirm their finding for an unoptimised geometry, but once the structural relaxations are taken into account, this exchange coupling changes its sign and implies the surface of CMO to have the same G-type antiferromagnetic order as in the bulk. However, the suggested SF can be induced in the system by introducing an excess of electrons.

MM 34.40 Tue 18:30 P4

Microstructure and Mechanical behavior of Copper-Iron Multilayers produced by Accumulative Roll Bonding — •Maher Ghanem, Benoit Merle, Heinz Werner Höppel, and Mathias Göken — Department of Materials Science and Engineering, Institute I, University of Erlangen-Nürnberg (FAU), Germany

The accumulative roll bonding (ARB) process has been applied recently to produce multilayer composites with grain sizes in the range of submicron to nanometer. Such multilayer composites show a good ductility with reported tremendous increases in strength as the grain sizes are refined down to the submicron range.

Laminated Cu/Fe Nanocomposite with alternating layers of Oxygen-free copper (OFC) (>99.99% pure) and pure iron (99.85%) were produced by accumulative roll-bonding (ARB). The Nanocomposite was successfully roll bonded with 50% reduction through the addition of a heat treatment step at 150°C after each pass. The process was performed up to 8 passes (N8). Microstructure of the nanocomposites was evaluated using scanning electron microscope in the backscattered mode (BSE-SEM). Mechanical properties were investigated through tensile and nanoindentation tests. Nanoindentation and tensile tests were performed in order to observe the changes in the mechanical properties of samples both locally and globally as the number of ARB passes increased.

MM 34.41 Tue 18:30 P4

Current status and future prospectives of the multi-purpose x-ray scattering beamline BL9 of DELTA — •Florian Otte, Jennifer Bolle, Michael Paulus, Christian Sternemann, and Metin Tolan — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund

We present the current status of the multi-purpose beamline BL9 of the synchrotron radiation source DELTA located at the TU Dortmund. The beamline is dedicated to (surface) x-ray diffraction, x-ray reflectivity and small angle x- ray scattering experiments with focus on soft matter research and materials science. Examples for study of protein adsorption, protein-protein interaction and structure formation in alcohols will be given. The upgrade of the beamline with a new wiggler source in 2018 will be discussed along with the implications for future experiments.

MM 34.42 Tue 18:30 P4

Observation of the influence of hydrogen on the phase transformation and fracturing behaviour of steel samples during tensile tests using synchrotron radiation — •Beate Pfretzschner, Axel Griesche, and Thomas Schaupp — Bundesanstalt für Materialforschung und -prüfung, Berlin, Deutschland

Hydrogen exhibits a detrimental influence on the mechanical properties of Fe-based alloys. The suggested mechanisms of hydrogen embrittlement are ambiguous and versatile. One of the effects of hydrogen in steels is its ability to change the phase transformation behaviour from austenite to martensite. In this work we present in-situ energy dispersive x-ray diffraction (ED-XRD) experiments performed on supermartensitic stainless steel samples with and without hydrogen during tensile tests. In order to perform ED-XRD scans, the path-controlled tensile test were paused every 0.25 mm. During these pauses spectra were acquired at seven positions on the sample along the tensile axis with a distance of 0.75 mm between each position. This procedure allows to follow the stress- or strain-induced phase transformation of the retained austenite to martensite in-situ. Simultaneous to the diffraction patterns, radioscopic images were acquired during the fracturing of the sample at a rate of 500 fps. Significant differences were observed in the phase transformation behaviour and the fracturing performance between hydrogenous samples and samples without hydrogen.

MM 35: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Time: Tuesday 18:30–20:30 Location: P2-OG4

MM 35.1 Tue 18:30 P2-OG4

Angular projection potentials for density functional calculations — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Development of advanced 21st century applications benefits from a quantum-mechanical understanding of material properties by density-functional theory. However, because the Kohn-Sham-Schrödinger equation must be solved numerically, for all but the smallest systems considerable computer resources are needed which makes very precise calculations difficult. In order to overcome this problem numerous techniques have been developed in the past to make the calculations affordable.

It is my aim to present a novel approach based on non-local potentials which act as projection potentials in the space of spherical harmonics. I will explain the unconventional mathematical techniques that can be used to prove that the Kohn-Sham-Schrödinger equation for these potentials can be solved exactly in the angular variables and, in view of the present computing capabilities, practically exactly in the radial variables. I will discuss the advantage of the use of angular projection potentials for precise total-energy calculations. The advantage arises from the fact that, as a consequence of the practically exact calculable density, the stationarity property of the total-energy functional with respect to the potential can be exploited to full extent.

MM 35.2 Tue 18:30 P2-OG4

DFPT within the All-Electron FLAPW Method: Application to Phonons — •Christian-Roman Gerhorst, Markus Betzinger, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In all-electron methods based on Density Functional Theory, typically the Finite Displacement approach is employed when describing the effect of a phonon perturbation on an electronic many-particle system. In difference to this common procedure, we implement the considerably more effective Density Functional Perturbation Theory (DFPT) into our full-potential linearized augmented plane-wave (FLAPW) code `FLEUR`; i.e. an all-electron code avoiding any approximation to the shape of the potential including the $1/r$ singularity. This is a non-trivial problem, because we have to tackle a position-dependent basis set generating additional Pulay and surface terms beyond the contributions known for force calculations when atoms are displaced. In this contribution, we report about the key challenge to the realization of the DFPT, which is the self-consistent solution of the Sternheimer equation providing the linear response of the electron density to a phonon perturbation. In a next step, we will use these results to construct the Dynamical Matrix encoding all relevant phonon information to shed light on the phonon-related properties of electronic many-particle systems.

MM 35.3 Tue 18:30 P2-OG4

Conceptual problemsof self-interaction corrections — •Charlotte Vogelbusch, Ronald Starke, and Lenz Fiedler — TU Freiberg, Institute for Theoretical Physics, Germany

Electronic structure calculations with density functional theory usually include the so-called self-interaction error which occurs due to the approximation of the exchange-correlation functional.

A corresponding self-interaction correction has first been introduced by J. P. Perdew and A. Zunger. This poster deals with the main aspects and problems of their method. In particular, we discuss the recent modification of the Perdew-Zunger self-interaction correction proposed by M. R. Pederson [2].

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

MM 35.4 Tue 18:30 P2-OG4

Numerical improvements of Fermi-Löwdin orbital self-interaction correction — •Lenz Fiedler, Torsten Hahn, Charlotte Vogelbusch, and Jens Kortus — TU Freiberg, Institute for Theoretical Physics, Germany

Electronic structure theory calculations based on density functional theory (DFT) using semilocal approximations for exchange and correlation are subjected to the self-interaction error. The recently proposed Fermi-Löwdin orbital method for self-interaction correction (FLOSIC) is based on sets of localized orbitals, that are a unitary invariant transformation of the Kohn-Sham orbitals [1,2]. The practical application of this method is however still numerically costly because one needs to determine the Fermi orbital descriptors that minimize the total energy. Numerical improvements to this optimization will drastically improve the performance of the whole FLOSIC DFT method.

We present the implementation of a preconditioned conjugate gradient [3] and a quasi-Newton L-BFGS algorithm [4] that draw on approximations of the analytical Hessian of the energy function. For a set of small molecules, benchmarks are done for different approximated Hessians. We here discuss the influence of different methods to approximate the Hessian and the usage of off-diagonal Hessian elements on the optimization performance.

[1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[2] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[3] D. Liu, J. Nocedal, Math. Prog. B 45, 503 (1989)
[4] W. Hager, H. Zhang, SIAM J. Optim., 16-1, 170 (2005)

MM 35.5 Tue 18:30 P2-OG4

Electronic and Magnetism Properties of Vacancy-Defected, Fluorine Doped and Adsorption upon MO3 (M= Cr, Mo, W) Surface: a first-principles study — •Masoud Mansouri[1,2] and Tahereh Mahmoodi[1] — [1]Department of Physics, Mashhad Branch, Islamic Azad University, Mashhad 9187147578, Iran — [2]Computational Science Unit, Research Center for Applied Biology, Mashhad Branch, Islamic Azad University, Mashhad, Iran

In this work, a systematic DFT calculation was carried out to investigate the effects of various kinds of dopants on the electronic structure of MO3 (M= Cr, Mo, W) Surface. The possibility to obtain magnetic phase from native defects in pure bulk is investigated. We found that vacancies can induce a magnetic phase of *2 μB with a local magnetic moment, whereas corresponding M vacancies (VM) provides the transition of the insulating MO3 into a metallic-like phase and changes the electronic transport. Moreover, We find that Fluorine (F) doping improves the metallic phase MO3*x Fx (x= 0.04, 0.08, 0.16), where the near Fermi states are formed mostly from M d-orbital and admixture of O-2p orbitals. Next, we present results on the influence of the common gas molecules (Ch4, H2S and NO2) on the electrical resistivity. The most stable configurations, magnetism, adsorption energies, Fermi surface and electronic properties are thoroughly discussed.

MM 35.6 Tue 18:30 P2-OG4

An Investigation of Group V dopants in Silicon using Linear Scaling DFT — •Jack Poulton and David Bowler — London Centre for Nanotechnology, 19 Gordon St, London, WC1H 0AH

The aim of our work is to model the incorporation and properties of group V element dopants in silicon using linear scaling density functional theory. In doing so we hope to learn how to incorporate new impurities and make predictions as to how the behaviour of these impurities for comparison with experimental data. This will then allow us to determine the suitability of certain dopants for usage as qubits in a silicon based solid state quantum computer.

MM 35.7 Tue 18:30 P2-OG4

Deciphering chemical bonding with Fermi-Löwdin orbitals — •Torsten Hahn[1], Sebastian Schwalbe[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore Maryland (MD), US

The recently developed Fermi-Löwdin orbital based method for the correction of the self-interaction error within Density Functional Theory (FLO-SIC) [1,2] does provide improved orbital eigenvalues and more realistic level ordering [3]. We demonstrate the versatility of this method to provide details of chemical bonding by applying it to several systems featuring both localized and delocalized multi-center chemical bonding.

We present results on systems with varying structural complexity: Boron clusters, compounds containing planar tetra-coordinated carbon as well as several aromatic and anti-aromatic molecules. The FLO-SIC method yields an inherently 'chemical' representation of bonding in terms of Lewis-type lone and binding electron pairs as well as delocalized multi-center, many-electron bonds. We anticipate that this parameter free methodology becomes a reliable tool to obtain insights into fundamental bonding details especially in situations where standard DFT fails.

[1] M. R. Pederson et.al, JCP 140, 121103 (2014).
[2] M. R. Pederson, JCP 142, 064112 (2015).
[3] T. Hahn et al., JCP 143, 224104 (2015).

MM 35.8 Tue 18:30 P2-OG4

Binding energy curves for diatomic molecules obtained by FLO-SIC DFT — •Simon Liebing[1], Sebastian Schwalbe[1], Torsten Hahn[1], Jens Kortus[1], and Mark Roger Pederson[2] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore, USA

The recently developed Fermi-Löwdin orbital method to correct the self-interaction error within DFT (FLO-SIC) [1,2] is used to study bond dissociation of diatomic molecules (e.g. N_2, O_2 and LiF). Binding energy curves are derived within this FLO-SIC methodology and the obtained results are compared to quantum chemical methods (RHF, UHF and ROHF in combination with CCSD/CCSD(T)). Due to the fact that FLO-SIC DFT recovers the correct -1/r behaviour of the potential, the obtained energies for large (infinite) separations agree well with the quantum chemical results. Further, changing Fermi orbital configurations as a function of the separation distance are observed. These distinct configurations could be interpreted as step-wise breaking of multiple bonds during the stretching of the considered molecule and corresponding alterations of spins within its electronic structure.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] T. Hahn et al., JCP, vol. 143, 224104 (2015)

MM 35.9 Tue 18:30 P2-OG4

Groundstates of the ternary clathrate $Ba_8Ni_xGe_{46-x-y}\square_y$ **obtained with an iterative cluster expansion approach** — •Martin Kuban, Santiago Rigamonti, Maria Troppenz, and Claudia Draxl — Humboldt-Universität zu Berlin

Intermetallic clathrates are promising candidates for the construction of thermoelectric (TE) devices. These rely on a junction between *n*- and *p*-type semiconductors. The clathrate compound $Ba_8Ni_xGe_{46-x-y}\square_y$ is of special interest, as it presents a crossover from *p*-type to *n*-type conductivity around $x = 4.0$ [1]. Thus, a junction on the same base material could be tailored. In this work, we perform an *ab-initio* study of the structural stability and electronic properties of this compound in the composition range $0 \leq x \leq 6$ and $0 \leq y \leq 4$. Both the substitutional species (Ni) and vacancies ($\square$) are treated on the same footing, through a cluster expansion (CE) in the quasi-ternary Ge/Ni/$\square$ sublattice. The large size of this sublattice (46 sites) leads to a combinatorial explosion of the number of configurations, i.e. the possible arrangements of the substitutional atoms and vacancies in the lattice. As this prevents the use of standard CE methodology, we make use of an iterative CE technique (iCE) as implemented in the code `CELL` [2]. The iCE is based on efficient samplings of the configurational space. The structural properties (lattice constants, bond distances, etc.) as well as the electronic bandstructure of the stable structures are analyzed.

[1] U. Aydemir *et al.*; Dalton Trans **44**, 7524 (2015).
[2] S. Rigamonti *et al.*, in preparation.

MM 35.10 Tue 18:30 P2-OG4

The inapplicability of exact constraints, and a minimal two-parameter DFT+*U* generalisation, for self-interaction error correction — •Glenn Moynihan[1], Gilberto Teobaldi[2,3], and David D. O'Regan[1] — [1]School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland. — [2]Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, U.K. — [3]Beijing Computational Science Research Center, China.

In approximate DFT, the self-interaction error (SIE) is a ubiquitous systematic inaccuracy responsible for underestimated insulating gaps, inaccurate dielectric properties and reaction barriers. It hinders the predictive applicability of DFT to spectroscopy, photochemistry, electrochemistry, and crystal-structure stability. It is, however, amenable to approximate correction using efficient methods such as DFT+U [1]. A calculation scheme for the Hubbard U parameters by variationally extremising a suitable functional might be desirable. but we show here that such an approach is not readily viable. Specifically, we prove that self-consistent constrained DFT [3] cannot be generalised for the non-linear constraints needed to target SIE [2]. We circumvent this using a generalised DFT+U functional, enabling the simultaneous correction of total-energies and ionization potentials, or either together with Koopmans' condition. For the latter, we outline a practical, approximate first-principles scheme by which the required Hubbard parameter pair, U_1 and U_2, may be estimated. [1] H. J. Kulik, et al., Phys. Rev. Lett. **97**, 103001 (2006). [2] Phys. Rev. B Rapid Comms., Accepted (2016), arXiv:1608.07320. [1] Phys. Rev. B **94**, 035159 (2016).

MM 35.11 Tue 18:30 P2-OG4

A Hubbard *U* based correction method for exciton binding in neutral excitations: TDDFT+*U* — •Okan K. Orhan and David D. O'Regan — School of Physics, Trinity College Dublin, Ireland.

The DFT+U (density-functional theory + Hubbard U) method is widely used to improve the approximate DFT description of the ground state properties of solids and molecules comprising transition-metal ions. We introduce its generalisation to the time domain in the guise of TDDFT+U (time-dependent DFT+U), intended to extend these improvements to the calculation of neutral excitations. Related methods have been previously discussed [1,2], and here we offer a detailed treatment emphasising single-particle excitations and absorption spectra. Our software implementation is a combination of the linear-scaling DFT+U [3] and linear-response TDDFT [4] functionalities available in the ONETEP code [5]. In a study of small nickel-comprising molecules, we find that the Hubbard U correction to the exchange-correlation kernel acts to partially cancel the effects of the DFT+U term of the underlying ground-state potential, enhancing the exciton binding.

[1] C.-C. Lee, H. C. Hsueh, and W. Ku, Phys. Rev. B **82**, 081106(R) (2010). [2] D. Shin, G. Lee, Y. Miyamoto, and N. Park, J. Chem. Theory Comput., **12** (1), pp 201-208 (2016). [3] D. D. O'Regan, N. D. M. Hine, M. C. Payne, and A. A. Mostofi, Phys. Rev. B **85**, 085107 (2012). [4] T. J. Zuehlsdorff, N. D. M. Hine, M. C. Payne, and P. D. Haynes, J. Chem. Phys. **143**, 204107 (2015). [5] C. K. Skylaris, P. D.

Haynes, A. A. Mostofi, and M. C. Payne, J. Chem. Phys., **122** (8), 084119 (2005). For the ONETEP code, see http://www.onetep.org

MM 35.12 Tue 18:30 P2-OG4

Implementation of Electron-Phonon Coupling in the KKR Formalism and its Applications to Simple Metals — Carsten Eberhard Mahr, •Michael Czerner, Christian Franz, and Christian Heiliger — Justus-Liebig-University, Giessen, Germany

Electron-phonon coupling is one of the main incoherent inelastic scattering mechanisms in a wide variety of crystalline material systems at room temperature. Therefore, it is necessary to incorporate those effects in any realistic calculation of thermoelectric properties. We do so by extending our density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

By approximating the Fröhlich-type interaction with a self-energy $\Sigma_{\mathrm{eph}} = -i\frac{\hbar}{2\tau}$ we are able to compute the dressed propagator G by solving Dyson's equation $G = G_{\mathrm{ref}} + G_{\mathrm{ref}} \cdot \left(\Delta V + \Sigma_{\mathrm{eph}}\right) \cdot G$, where G_{ref} is the Green's Function of an arbitrary (though typically repulsive) reference system. The corresponding electron-phonon scattering time τ is extracted from electron linewidth calculations.

We demonstrate the physical validity of the beforementioned calculational scheme for non-equilibrium properties by comparing evaluated temperature dependent resistivity characteristics of transport systems consisting of copper, aluminum and other simple metals to experiment. Further, technical details of the implementation in the KKR basis set are presented.

MM 36: Invited talk Curtin

Time: Wednesday 9:30–10:00 Location: BAR 205

Topical Talk MM 36.1 Wed 9:30 BAR 205

Theory Driven Data Driven Design for Structural Metals — •William A. Curtin — Laboratory for Multiscale Mechanics Modeling, Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland

A fundamental idea of data-driven design of materials is that the design goal can be adequately represented by some descriptors that, in turn, can be computed by first-principles methods or estimated. For structural metals, the design goals are quantities such as yield strength, work hardening, and toughness or ductility, which are often a function of temperature and strain rate. The quantities that are most amenable to first-principles computations are zero-temperature elastic and lattice constants, solute misfit volumes, stacking fault energies, solute interactions stacking faults, solute diffusion coefficients, and stable precipitate structures and properties. Few theories quantitatively connect design goals to computable quantities and for structural materials, there is thus an urgent need for theory-driven data-driven design. This talk will present two examples of theory-driven-data-driven design, wherein a fundamental theory is developed, reduced to computable quantities, validated, and then used to guide material selection for enhanced mechanical performance.

MM 37: Topical session: Data driven materials design - defect engineering

Time: Wednesday 10:15–11:45 Location: BAR 205

Topical Talk MM 37.1 Wed 10:15 BAR 205

Data-driven theory-guided materials design containing scale-bridging concepts — •Martin Friák[1,2,3], Stefanie Sandlöbes[4,3], Zongrui Pei[3], David Holec[5], Mojmír Šob[2,1,6], Jörg Neugebauer[3], and Dierk Raabe[3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [4]Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany — [5]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [6]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Ab initio based calculations combined with scale-bridging models have recently emerged as powerful tools in modern materials design. Their further enormous progress has just started thanks to the recent onset of open-access databases with quantum-mechanical results. The talk will provide selected examples of materials development based on data-driven analysis, its combination with traditional concepts (e.g., CALPHAD) and experimental verification. The theory-guided materials design will be exemplified by the case of novel ductile Mg-based alloys assessed by pattern extraction, introduction of generalized descriptors, and multi-dimensional search for optimum compositions. Further, the development of new superalloys employing open-access databases will illustrate the need of their critical cross-validation against experiments.

MM 37.2 Wed 10:45 BAR 205

SEGROcalc, a computational toolbox and database for grain-boundary engineering — Daniel Scheiber, Anatol Drlicek, Nada Kulo, Jürgen Spitaler, Vsevolod Razumovskiy, and •Lorenz Romaner — Materials Center Leoben Forschung GmbH, Roseggerstasse 12, 8700 Leoben, Austria

Segregation of solute elements to grain boundaries (GBs) is a key factor affecting production and performance of many technologically relevant materials. It influences fundamental material properties such as formability, crack propagation, grain growth, precipitation, diffusivity or electric conductivity. By controlling the segregation state, a lever for developing materials of superior properties can be obtained. In this talk we present the development of SEGROcalc, a software for inspecting segregation at GBs and estimating the impact of segregation on materials properties. The basis for the software is formed by a database where a vast amount of literature values of segregation energies and strengthening energies are collected together with the necessary metadata providing information about material, GB structure, segregation site, literature source, or method. The method includes density functional theory calculations, phenomenological modeling and experimental data. The database is accessible via a graphical user interface which allows analyzing the database entries, monitor GB structure, compare segregation energies from different sources, identify solutes beneficial for GB strength and estimate chemical composition of the GB. Representative examples will be shown and the current level of agreement between different theoretical models and experiment discussed.

MM 37.3 Wed 11:00 BAR 205

Efficient sampling in materials simulation - Exploring the parameter space of grain boundaries — Josua Gösmann[1], Christian Greiff[1], Holger Dette[1], and •Rebecca Janisch[2] — [1]Department of Mathematics, Institute of Statistics, Ruhr-Universität Bochum, Germany — [2]ICAMS, Ruhr Universität Bochum, Germany

High-throughput numerical simulations as well as experiments allow a systematic variation of individual parameters, such as e.g.composition, and the coverage of a broad range of these parameters. Nevertheless, the majority of properties that are available today are so-called intrinsic properties like stability, stiffness, or band gaps. Extrinsic properties, like interface distribution functions, energies or mobilities, are less frequently available. As a matter of fact, because they depend on several variables at the same time, such properties form multidimensional databases of their own for one particular material. For such cases we want to promote an efficient sampling of the variable space that is based on design of experiment principles. As a suitable example we pick grain boundary energies, which depend on five geometric degrees of freedom.

We introduce two methods to improve the current state of the art. Based on an existing energy model the location and number of the energy minima along which the hierarchical sampling takes place is predicted from existing data points without any a-priori knowledge, using a predictor function. Furthermore we show that in many cases it is more efficient to use the above mentioned sequential sampling, rather than sampling all observations homogeneously in one batch.

MM 37.4 Wed 11:15 BAR 205

Environmental tight-binding modelling of structural defects in metals — •Eunan J. McEniry, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The modelling of structural defects in metallic systems, such as phase boundaries and dislocations, involves a complex interplay between the chemical composition and the local atomic coordination. Specific challenges include the role of incoherency, the preferential segregation of light elements such as carbon and hydrogen to such defects, and the need to efficiently describe the interactions of compositionally complex systems. While the chemical complexity can be described accurately within density functional theory approaches, the computational cost becomes prohibitive when studying, for example, hydrogen segregation to incoherent phase boundaries between a host matrix and a precipitate.

The environmental tight-binding approach offers a rigorous and computationally efficient framework in which high-throughput atomistic simulations of multi-component systems can be performed, which retains the full quantum-mechanical nature of the problem. The development of potentials derived from this approach will be illustrated, demonstrating the flexibility and speed of the method. As an example, the energetics and diffusion behaviour of hydrogen at the incoherent phase boundary between α-Fe and TiN will be presented.

MM 37.5 Wed 11:30 BAR 205

The shear instability energy as a new parameter to characterise deformation behaviour of materials — Mansour Kanani[1], Alexander Hartmaier[2], and •Rebecca Janisch[2] — [1]School of Mechanical Engineering, Shiraz University, Iran — [2]ICAMS, Ruhr-Universität Bochum, Germany

Systematic relationships between a limited number of fundamental material properties and the observable behaviour of a material are needed for successful design of new materials. To this purpose we introduce the shear instability energy Γ as a new materials parameter. Using interfaces in lamellar TiAl as a case study, we show that Γ can link stacking fault energies from a quasistatic (e.g. ab initio density functional theory based) calculation with the deformation mechanisms that are observed in a molecular dynamics simulation of shear.

Furthermore the shear instability energy can be used to scale between the results of calculations with different interatomic potentials, i.e. also to evaluate trends in deformation mechanisms across different elements. In this, the concept of the shear instability energy is more comprehensive than models which rely only on the ratio of unstable and stable stacking fault energies. This makes it a promising tool for enhancing high-throughput characterization of materials.

MM 38: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - defects, structure and thermodynamics

Time: Wednesday 10:15–11:30 Location: IFW A

MM 38.1 Wed 10:15 IFW A

Structure, thermodynamics and Li storage of and in amorphous siliconoxycarbides: insights from first-principle calculations — •Jochen Rohrer and Karsten Albe — FG Materialmodellierung, FB Material- und Geowissenschaften, Technische Universität Darmstadt

Precursor-derived amorphous siliconoxycarbides (SiOC) are attracting increased attention as potential anode material for Li-ion batteries. Capacities of 600 mAh/g and above have been achieved. Furthermore, SiOCs have been reported to be thermodynamically stable relative to the crystalline boundary phases cristobalite, SiC and graphite. On the microscale, SiOCs are well characterized and can be described by regions consisting of amorphous SiO_2, graphitic free carbon and mixed ternary regions. The details of the atomic structure within the ternary regions are, however, still under debate.

In this contribution we present strategies to model and determine local atomic characteristics of SiOC using density functional theory calculations. Using cluster models, we systematically investigate the bonding environment of carbon in ternary Si-O-C regions. Thereby we consider various coordinations and the possibility of hydrogen incorporation into the amorphous network [1]. Based on the predicted local C environment, we then design periodic supercell models with variable carbon content, compute thermodynamic stability and investigate Li storage in a way similar to our previous work on Si anodes [2].

[1] J. Rohrer et al., *submitted to Int. J. Mater. Res.* (Nov 2016).

[2] J. Rohrer and K. Albe, *J. Phys. Chem.* C **117**, 18796 (2013).

MM 38.2 Wed 10:30 IFW A

Oxygen Defects in LTO – Structural Models and Adapted DFT Treatments — •Markus Schuderer, Karsten Reuter, and Christoph Scheurer — Technische Universität München, Germany

$Li_4Ti_5O_{12}$ (LTO) receives increasing interest as a zero-strain anode material for lithium ion batteries. One route pursued to improve its limited electronic conductivity is via the deliberate introduction of oxygen defects during synthesis. Little is presently known though, whether these defects enrich at the electrode-electrolyte interface and concomitantly contribute to structural or charge transfer limitations. Aiming to contribute to this context from the perspective of first-principles electronic structure calculations, we assess differing setups in terms of reliability and computational efficiency. This comprises a comparison of periodic supercell and solid-state embedded cluster approaches, as well as treatments on the semi-local or screened hybrid level of density-functional theory. While semi-local functionals delocalize the excess charge density associated with the defect and lead to metallic systems, the hybrid functional recovers the experimentally observed band gap and localizes the charge density on titanium ions directly coordinating the defect. We show that this localization can already be appropriately captured with small embedded clusters, rendering this approach numerically far more efficient in particular for studies of surface or interface defects.

MM 38.3 Wed 10:45 IFW A

Ion channelling contrast to reveal structure and growth behaviour of $LiNi_{0.5}Mn_{1.5}O_4$ battery materials — •Manuel Mundszinger[1], Tobias Wälde[1], Jörg Bernhard[1], Michael Kinyanjui[1], Marilena Mancini[2], Peter Axmann[2], Margret Wohlfahrt-Mehrens[2], Ute Golla-Schindler[1], and Ute Kaiser[1] — [1]Ulm University, Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Helmholtzstrasse 8, 89081 Ulm

Ion channelling contrast [1] was utilized to characterize the crystallinity and crystalline architecture of $LiNi_{1.5}Mn_{0.5}O_4$ particles [2] for battery cells. The $LiNi_{0.5}Mn_{1.5}O_4$ particles were cut by the focused ion beam (FIB) machine; then the FIB was used to produce channelling contrast revealing the polycrystallinity of the material, allowing to determine grain size distribution and architecture. For systematic investigations, differently sized particles (10-30 micrometre in diameter) were examined. We found that with increasing particle size the number and the average size of the grains increases. This allows to conclude that during growth new grains are formed as well as existing grains grow. SAED and HRTEM reveal that the structure is cubic. Ion channelling contrast and EBSD contrast were compared showing very similar results. This work was done in the LiEcoSafe project funded by the BMBF (03X4636C).

[1] C. A. Volkert et al, MRS Bulletin, 32:389-399, 5, 2007.

[2] P. Axmann et al, Journal of Power Sources 301 (2016) 151-159.

MM 38.4 Wed 11:00 IFW A

Modeling occupational disorder in $Li_4Ti_5O_{12}$ battery materials: Intrinsic complexity and its effect on ion mobility — •Hendrik H. Heenen, Christoph Scheurer, and Karsten Reuter — Technische Universität München, Germany

Lithium-titanium-oxide ($Li_4Ti_5O_{12}$, LTO) is unique among battery materials due to its exceptional cyclability and high rate capability.

This performance is assumed to derive at least partly from the occupational disorder introduced via mixed Li/Ti occupancy in the LTO spinel-like structure. Notwithstanding, the exact atomic-scale influence of this disorder on Li ion mobility remains an open question.

We explore the vast configuration space accessible during high-temperature LTO synthesis by Wang-Landau sampling. Use of a numerically efficient, density-functional theory validated interatomic potential [1] allows for extensive sampling in simulation cells large enough to appropriately capture the long-range disorder. The determined configurational ensemble is indeed characterized by a large degree of microscopic inhomogeneity. Subsequent room-temperature molecular dynamics simulations reveal the dominant fraction of Li ions in this ensemble to be immobile on nanosecond timescales. However, certain disorder motifs give rise to a novel correlated ion diffusion mechanism. We discuss this mechanism in the context of the evolution and morphology of the so-called two-phase reaction appearing during Li intercalation [2].

[1] M. Vijayakumar *et al.*, J. Power Sources **196**, 2211 (2011)
[2] M. G. Verde *et al.*, ACS Nano **10**, 4312 (2016)

MM 38.5 Wed 11:15 IFW A

Ab initio modeling of Li-rich transition metal oxyfluorides — •Holger Euchner[1] and Axel Gross[1,2] — [1]Helmholtz Institute for Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm — [2]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

Recently, Li-rich transition metal (TM) oxyfluorides, were identified as promising electrode materials in Li-ion batteries [1,2]. Due to the evidenced robustness of the underlying framework – a disordered rock salt structure (DRS), consisting of two disordered fcc sublattices, exhibiting TM/Li and O/F disorder, respectively – this class of materials is a potential candidate for future application in Li-ion technology.

To provide insight into underlying mechanisms and potential for improvement, we have conducted a computational study of a number of $\mathrm{Li}_x\mathrm{TM}_{1-x}\mathrm{O}_y\mathrm{F}_{1-y}$ compounds. Using periodic density functional theory calculations, the impact of different TMs as well as different O/F concentrations on structural stability, (de-)lithiation behavior and Li diffusion is investigated. Apart from predicting open circuit voltage and energy density, we present an analysis of Li-diffusion pathways and corresponding barriers, which we relate to local environment and bonding characteristics of Li atoms.

[1] R. Chen et al., Adv. Energy Mater. **5**, 9 (2015).
[2] S. Ren et al., Adv. Sci. **2**, 10 (2015).

MM 39: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and deformation III

Time: Wednesday 10:15–11:15 Location: IFW B

MM 39.1 Wed 10:15 IFW B

Glass formation by severe plastic deformation of crystalline Cu/Zr nano-layers — •Suzhi Li[1], Lars Pastewka[2,3], and Peter Gumbsch[2,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, 79108 Freiburg, Germany

The deformation of crystalline Cu/Zr nano-layers under severe shearing was studied by using molecular dynamics simulations. The whole process can be divided into two distinct stages. The early stage of plasticity is governed by dislocations. The dislocation-interface interaction can induce the interface roughening and slow mechanical mixing around boundaries. As strain is further applied, dislocation activities become less active. Under the large strain, domains are further refined and finally the interfaces are attached locally, where solid-state crystal-to-amorphous transition occurs. The deformation mode then transforms from dislocation plasticity to amorphization. The following deformation is fully localized in the glass transition zone where a strong atomic mixing takes place. The whole crystal-to-amorphous transition process can be characterized by certain Voronoi cells, such as Cu-centered <0 0 12 0>. In addition, the amorphization in thinner layers can be achieved at smaller shear strain. Our work enriches the understanding of amorphization and mechanical alloying in heavily deformation multicomponent systems.

MM 39.2 Wed 10:30 IFW B

Micro-mechanics of amorphous metal/polymer hybrid structures with 3D cellular architectures: size effects, buckling behavior and energy absorption capability — •Maxime Mieszala[1], Laszlo Petho[1], Johann Michler[1], Madoka Hasegawa[1], Jens Bauer[2], Oliver Kraft[2], and Laetitia Philippe[1] — [1]Empa, Materials Science and Technology, Thun, Switzerland — [2]Karlsruhe Institute of Technology, Institute for Applied Materials, Karlsruhe, Germany

By designing advantageous cellular geometries and combining the material size effects at the nanometer scale, lightweight hybrid micro-architectured materials with hierarchical cellular structures and tailored structural properties are achieved. To determine the mechanical performance of polymer cellular nanolattices reinforced with a metal coating, 3D laser lithography and electroless deposition of an amorphous layer of NiB is used to produce metal/polymer hybrid structures. Microcompression experiments show an enhancement of the mechanical properties with the thickness of the NiB layer, suggesting that the deformation mechanism and the buckling behavior are controlled by the size induced brittle-to-ductile transition in the NiB layer. In addition, the energy absorption properties demonstrate the possibility of tuning the energy absorption efficiency with adequate designs.

MM 39.3 Wed 10:45 IFW B

Impact of the composition of Au-Ag alloys on the mechanical properties of dealloyed nanoporous gold — •Birthe Müller[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Nanoporous gold (NPG) made by dealloying can be viewed as a nanofoam that consists of interconnected nanoscale pores and solid "ligaments" that can take the shape of macroscopic bodies. Due to its tunable feature size from a few to a several hundred nanometers and its high chemical stability NPG has proven an attractive model system for various small scale studies. E.g. the mechanical properties of NPG have been the subject of a multitude of studies over many years. Analog to macroscopic metallic foams, results are frequently linked to the solid fraction, ϕ. Focusing on ϕ, the influence of the initial composition of precursor alloy and the manufacturing methods are often neglected.

We present a comparative study on the mechanical properties of NPG using varying initial compositions and different processing procedures. $\mathrm{Au_xAg_{100-x}}$ precursors with $x = 20, 25, 30, 35$ were synthesized via electrochemical dealloying in 1 M $\mathrm{HClO_4}$ as well as free corrosion in concentrated $\mathrm{HNO_3}$. Using compression tests with single loading and load/unload protocols we investigate the stress-strain behavior, the Young's modulus and the Poisson's ratio. We find significant differences in the mechanical responses that contradict the image of a ϕ controlled behavior.

MM 39.4 Wed 11:00 IFW B

Interfaces and Vortices under High Pressure Torsion — •Roman Kulagin[1], Yulia Ivanisenko[1], Yan Beygelzimer[2], Andrey Mazilkin[1,3], Boris Straumal[1,3], and Horst Hahn[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Donetsk Institute for Physics and Engineering, NASU, Ukraine — [3]Institute of Solid State Physics RAS, Russia

Here we report our results on the behavior of interfaces in the layered metallic samples under high pressure torsion (HPT). We found the development of plastic instabilities in initially flat layers during HPT and the formation of folds and vortices.

These phenomena cannot be explained by the Kelvin-Helmholtz instability mechanism. An important condition to observe the Kelvin-Helmholtz instability is that in the flowing matter the forces of inertia are of the same order of magnitude as the internal forces due to the atomic (or molecular) interactions. In this context in metal under plastic flow a role of such internal forces play forces related to flow stress. However, it is known that at moderate strain rate deformation the forces of inertia are significantly lesser than these associated with flow stress.

Using Finite Element Modeling we show that the formation of vortices during the HPT deformation occurs when the simple shear velocity field is blocked locally within the layers, or at the interfaces. As a result, the rotation of the material takes place on macroscopic level, i.e. the formation of the vortices is observed.

MM 40: Transport III - thermal transport

Time: Wednesday 10:15–11:15 Location: IFW D

MM 40.1 Wed 10:15 IFW D

TUNING QUANTUM ELECTRON AND PHONON TRANSPORT IN 2D MATERIALS BY STRAIN ENGINEERING: A GREEN'S FUNCTION BASED STUDY

— •Leonardo Medrano Sandonas[1,2], Rafael Gutierrez[1], Alessandro Pecchia[3], Gotthard Seifert[4], and Gianaurelio Cuniberti[1,5,6] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Consiglio Nazionale delle Ricerche, Rome, Italy — [4]Institut für Physikalische Chemie und Elektrochemie, Dresden,Germany — [5]Dresden Center for Computational Materials Science, Dresden, Germany — [6]Center for Advancing Electronics Dresden, Dresden, Germany

In the present work, using a DFTB method in combination with Green's function approaches, we address strain engineering of the transport setup (contact-device(scattering)-contact regions) on the electron and phonon transport properties of 2D materials, focusing on hBN, phosphorene, and MoS_2 monolayer. Considering unstretched contact regions, we show that the electronic bandgap displays an anomalous behavior and the thermal conductance continuously decreases after increasing the strain level in the scattering region. However, when the whole system (contact and device regions) is homogeneously strained, the bandgap for hBN and MoS_2 monolayers decreases, while for phosphorene first increases and then tends to zero with larger strain levels. Additionally, the thermal conductance shows a specific strain dependence for each of the studied 2D materials.

MM 40.2 Wed 10:30 IFW D

Ab initio investigation of the anomalous phonon softening in FeSi

— •Robin Stern[1] and Georg K. H. Madsen[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Institute of Materials Chemistry, TU Wien, Austria

The anomalous softening of the acoustic phonon peak in FeSi has recently received considerable experimental attention. In our work, we investigate the effect of thermal disorder on the lattice dynamics and the filling of the narrow band gap of FeSi using density functional theory. We show, by comparing the phonon density of states from temperature-independent and temperature-dependent force constants, that thermal structural disorder together with thermal expansion explains the anomalously strong renormalization of the acoustic phonons. Furthermore, we find an intricate interplay between thermal disorder and volume in gap closure.

MM 40.3 Wed 10:45 IFW D

Point defect phonon scattering and thermal conductivity in Silicon

— •Bonny Dongre and Georg K. H. Madsen — Institute of Materials Chemistry, TU Wien, Getreidemarkt 9/165, 1060 Wien, Austria

Due to the ever decreasing size of devices and increasing operating speeds, understanding and control of the thermal transport has gained paramount importance. Predicting the thermal conductivity of such devices is an inherent multi-scale problem. This requires full description of thermal transport behavior on electronic level, atomistic and mesoscopic structure levels.

The aim of the present work is to systematically analyze the effect of various types of defects, e.g. vacancies, interfaces and dislocations inevitably present in engineering materials, on their thermal conductivities. When viewed from the atomistic scale, quantitative description of phonon scattering strength can be obtained using inputs from ab intio methods like DFT. We have used the atomic-green's-function approach to calculate the scattering rates which are then fed into the Boltzmann transport equation to get the required thermal conductivity in Vacancy Si (Vac_{Si}) and Germanium substitutional (Ge_{Si}) defect systems.

We acknowledge support from EU Horizon 2020 grant 645776 (ALMA) (www.almabte.eu)

MM 40.4 Wed 11:00 IFW D

Topological nodal line Dirac semimetal HfSiS

— •Chandra Shekhar, Nitesh Kumar, Kaustuv Manna, Yanpeng Qi, Shu-Chun Wu, Binghai Yan, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Topological semimetals provide a wide platform to realize Dirac, nodal Dirac and Weyl fermions. Recently, HfSiS has been predicted as a nodal line Dirac semimetal. This compound shows hole carrier density which is higher as compare to the other known semimetals at 2K and massive amplitude of de Haas-van Alphen and Shubnikov-de Haas oscillations up to 30 K in 7 T. Low effective mass of the charge carriers acquire extra -Berry phase, a witness of topological Dirac type dispersion of bands which are originated from Si square net and Zr atoms. Furthermore, we establish the 3D Fermi-surface that consists of water caltrop-like electron and barley seed-like hole pockets. Asymmetrical nature of pockets is accountable to anisotropic magnetoresistance in HfSiS.

MM 41: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV

Time: Wednesday 10:30–13:00 Location: GER 38

Invited Talk MM 41.1 Wed 10:30 GER 38

Electronic excitations in 2D materials and heterostructures

— •Kristian Sommer Thygesen — Technical University of Denmark, Lyngby, Denmark

Atomically thin two-dimensional (2D) materials have recently emerged as a new class of materials with unique and highly tunable optoelectronic properties. Different 2D crystals can be stacked to form van der Waals heterostructures (vdWH) where the individual 2D layers are held together by weak van der Waals forces leading to atomically well-defined interfaces. This fascinating scenario opens up the possibility of designing heterostructures with tailored electronic or optical properties. I will give a general introduction to the electronic properties of 2D materials, including characteristic features of their dielectric screening and collective excitations with special emphasis on the challenges related to their ab-initio description. I will show how the dielectric function of a given 2D material can be controlled by embedding it into a vdWH, and how this in turn can be used to control the band structure, exciton binding energies or the plasmon dispersion in 2D materials.

MM 41.2 Wed 11:00 GER 38

Charge and energy transport at the nanoscale: A DFT perspective

— •Florian G. Eich, Fabio Covito, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Understanding the interplay between charge and energy transport at the nanoscale paves the way for novel thermoelectric devices, which may prove useful for the development for sustainable energy sources.

However, concepts, such as heat flow, temperature and entropy are only well-established at the macroscopic level for slow dynamics. This raises the question about whether these concepts can be employed for small length and short time scales. We will present our recent efforts to use a time-dependent density-functional theory framework, dubbed nonequilibrium thermal DFT, in order to generalize temperature and heat or energy flow to the microscopic regime. To this end we will highlight the analogy of the formally exact microscopic equations of motion for charge density and energy density in thermal DFT to the macroscopic equations of motion of hydrodynamics. Furthermore, we will present first result using our approach to compute transient energy energy currents induced by a temperature gradient and show that in the steady-state limit persistent temperature oscillations develop.

MM 41.3 Wed 11:15 GER 38

Conductance of aromatic and antiaromatic molecular circuits — Narendra P. Arasu and •Héctor Vázquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Molecular structures with delocalized conjugated orbitals play an essential role in molecular transport due to their high conductance and small attenuation factors. While much work has been done on aromatic molecules, some studies have shown that conductance actually decreases with aromaticity [1].

In this talk I will discuss the effect of (anti)aromaticity on conductance. I will show results of first-principles transport calculations for an aromatic-antiaromatic pair of molecules and compare with experiment. Conductance is calculated using DFT and NEGF including corrections to the DFT level positions. The corrected conductance values are in very good agreement with experiment. We find that the conductance of the antiaromatic molecule is much higher than that of its aromatic counterpart. Calculations show this to be a consequence of the smaller HOMO-LUMO gap of the antiaromatic complex as well as on the molecular level alignment at the junction [2].

[1] W. Chen, H. Li, J.R. Widawsky, C. Appayee, L. Venkataraman, and R. Breslow, J. Am. Chem. Soc. 136 918 (2014).

[2] S. Marqués-González, S. Fujii, J.-Y. Shin, H. Shinokubo, N.P. Arasu, H. Vázquez and M. Kiguchi, (to be submitted).

MM 41.4 Wed 11:30 GER 38

Current-induced cooling of Carbene-based molecular junctions: role of electrodes structure — •Giuseppe Foti and Héctor Vázquez — Institute of Physics, Czech Academy of Sciences Cukrovarnicka 10, Prague 6

In this talk I will present our first principles calculations based on density functional theory (DFT) plus Nonequilibrium Green's functions (NEGF) of the current-induced heating and cooling dynamics of a series of Carbene-based molecular junctions [1]. I will show how the atomistic details of electrode terminations have a strong impact on the heating dynamics of the junctions and how they can maximize the cooling of the system. In the cases where the molecule is attached to blunt leads and the electronic coupling to bulk states is strong the cooling efficiency of the most active vibrational modes decreases monotonically as bias increases. This results in the heating of the junction. On the other hand, when the molecule is connected to sharp electrode terminations such as chain-like structures, which can be formed experimentally when the metal-molecule bond is mechanically strong, and the electronic coupling to electrode states is weak, the cooling efficiency shows a non-monotonic behavior. It first decreases as a function of voltage but then increases at relatively high biases, effectively cooling down the junction [2]. These results reveal the important role of the atomistic structure of metal-molecule interface in the current-induced damping of localized molecular vibrations.

[1] Foti, G.; Vázquez, H. Nanotechnology 2016, 27, 125702.

[2] Foti, G.; Vázquez, H. submitted

MM 41.5 Wed 11:45 GER 38

DFTB-based recursive Green's function algorithms for electron transport in quasi-1D systems — •Fabian Teichert[1,2,4], Andreas Zienert[3,4], Jörg Schuster[4], and Michael Schreiber[2] — [1]Dresden Center for Computational Materials Science (DCMS), Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Within the last decades, quantum transport theory and density functional theory have become very important for predicting the electronic properties of new materials and future electronic devices.

We focus on the problem of improving quantum transport algorithms for large quasi-1D systems which are enormously time-consuming today. We combine the density functional tight binding (DFTB) approach with the recursive Green's function formalism (RGF), which is very effective for such systems. First, we show how to improve the RGF for the case of randomly distributed real defects. For this, we use the steps of the renormalization decimation algorithm (RDA), which is part of the electrode calculation. Second, we show how to improve the calculation of the surface Green's functions of electrodes which have a long unit cell. Here, we employ the decimation technique to reduce the dimensionality of the periodic Hamiltonian matrix, leading to effective matrices, which are treated by the RDA. Finally, we apply these algorithms to carbon nanotubes and present our results.

MM 41.6 Wed 12:00 GER 38

Conditions for formation of two-dimensional electron gas at the $LaFeO_3/SrTiO_3$ — •Igor Maznichenko[1], Sergey Ostanin[1], Arthur Ernst[2], Ingrid Mertig[1,2], Katayoon Mohseni[2], Holger L. Meyerheim[2], Eberhard K.U. Gross[2], Pengfa Xu[3], Wei Han[3], Philip M. Rice[3], Jaewoo Jeong[3], Mahesh G. Samant[3], and Stuart S.P. Parkin[2,3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [3]IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA

The formation of a conducting two dimensional electron gas (2DEG) at the interface between two insulating oxide layers was explained theoretically for atomically and chemically abrupt interfaces via polar discontinuity.

Here we show that a 2DEG is formed at the interface between thin layers of lanthanum ferrite, $LaFeO_3$ (LFO), that are more than 3 unit cells thick, when grown epitaxially on $SrTiO_3$ (STO) (001). The interface property highly depends on the surface property of TiO_2 terminated STO. The interface is conducting if the STO is not annealed in an oxygen environment prior to the LFO growth, while insulating if the STO is annealed.

First principles calculations reveal that a 2DEG should be realized for an ideal interface but that modest chemical intermixing suppresses it. These calculations also show that the presence of oxygen vacancies supports 2DEG formation due to electronic doping.

MM 41.7 Wed 12:15 GER 38

Thermal Renormalization of the Electronic Structure: Trends across Chemical and Structural Space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Advances in electronic structure theory now allow us to compute the renormalization of the electronic structure due to thermal nuclear motion from first principles [1]. In this work, we present a systematic computational assessment of this renormalization for 82 octet binaries in both the zincblende and the rocksalt structure. After validating our computational approach that is based on finite-differences [2] and Fröhlich-type corrections [3] for polar materials, we discuss and analyze the observed trends: For instance, we find that most materials exhibit the expected band-gap reduction upon temperature increase; however, some materials (e.g. CuCl and CdO) do not follow this trend and exhibit the opposite behavior. We discuss the underlying electronic mechanism as well as its dependence on the chemical composition and structure of the material. In this context, also the sensitivity of such calculations with respect to the chosen basis set and exchange-correlation functional (LDA, PBE, HSE06) are critically investigated.

[1] F. Giustino, arXiv:1603.06965 (2016).

[2] G. Antonius, *et al. Phys. Rev. Lett.* **112**, 215501 (2014).

[3] J. P. Nery and P. B. Allen, *Phys. Rev. B* **94**, 115135 (2016).

MM 41.8 Wed 12:30 GER 38

Spin-wave excitations and electron-magnon scattering from many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We study the spin excitations and the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory as implemented in the full-potential linearized augmented-plane-wave method. Starting from the GW approximation we obtain a

Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone theorem and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the non-interacting one, leading to a substantial improvement of the Goldstone-mode condition [1]. Finally, we employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy. We also see kinks in the electronic bands, which we attribute to electron scattering with spatially extended spin waves.
[1] Müller *et al.*, Phys. Rev. B **94**, 064433 (2016).

MM 41.9 Wed 12:45 GER 38

Charged supercells revised: Small Polarons in Oxides with proper account for long-range polarization — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Formation of small polarons (excess charges localized within one unit cell) often determines charge mobility and optical absorption in oxide materials. In this work, we address two important challenges in the DFT description of small polarons: sensitivity to the errors in exchange-correlation (XC) treatment and finite-size effects in supercell calculations. The polaron properties are obtained using a modified neutral potential-energy surface (PES) [1]. Using the hybrid HSE functional and considering the whole range $0 \leq \alpha \leq 1$ of exact exchange, we show that the modified PES model significantly reduces the dependence of the polaron level and binding energy in MgO and TiO_2 on the XC treatment. It does not eliminate the dependence on supercell size. Based on Pekar's model [2], we derive the proper long-range behavior of the polaron and a correction that allows to obtain the polaron properties in the dilute limit (tested for supercells containing up to 1,000 atoms). The developed approach reduces drastically the computational time for exploring the polaron PES, and gives a consistent description of polarons for the whole range of α. It allows us to find a self-trapped hole in MgO that is noticeably more stable than reported previously.—[1] B. Sadigh *et al.*, PRB **92**, 075202 (2015); [2] S.I. Pekar, ZETF **16**, 335 (1946). This work received funding from the Leibniz ScienceCampus "GraFOx".

MM 42: Topical session: Data driven materials design - high through-put

Time: Wednesday 12:00–13:15 Location: BAR 205

Topical Talk MM 42.1 Wed 12:00 BAR 205

Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials — •Alfred Ludwig — Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum

The design of new materials is a key challenge in materials science: e.g. new materials for future energy systems are urgently needed. Thin film combinatorial materials science (CMS) enables an efficient generation of consistent and large datasets on (unexplored) multinary materials systems, which promotes the discovery and optimization of new materials. CMS comprises the fabrication and processing of thin film materials libraries by combinatorial sputter deposition processes and optional post-deposition treatments, followed by extensive high-throughput characterization of the thin film samples contained in these libraries. The large datasets which are produced by the combinatorial approach need to be analyzed with new software tools, e.g. for the rapid mapping of phase diagrams. Obtained results for ternary and quaternary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover and discuss examples of the combinatorial development of intermetallic materials for superalloys and thermoelectric applications as well as the development of metal oxide thin film materials libraries for solar water splitting.

MM 42.2 Wed 12:30 BAR 205

Towards multi-scale high-throughput calculations of thermal and mechanical properties in transition-metal alloys — •Alessandro Lunghi, Stefano Sanvito, and David D. O'Regan — School of Physics, CRANN and AMBER, Trinity College Dublin, Dublin 2, Ireland

The discovery of advanced materials with targeted properties is a long-standing challenge, where computational material science is adopting an increasingly central role in establishing stable stoichiometries and property trends. The high-throughput approach is a particularly promising strategy [1], involving the calculation of specific properties of interest over combinatorial numbers of crystallographic structures. In this work, we demonstrate the high-throughput simulation of the mechanical properties for binary alloys of the form $Au_{1-x}M_x$, where M is a generic transition metal element. We have used the AFLOW repository [2] to generate more than 5000 equilibrium structures, from which we have re-relaxed and calculated the complete elastic tensor using Quantum Espresso [3]. We also show preliminary results on the development of a new methodological framework, in which, for example, the large data corpus produced during the latter screening initiative have been used to optimize empirical force fields suited for the calculation of thermal properties. This tool opens up the new possibility of extend high-throughput methods beyond system size limits of conventional DFT. [1] S. Curtarolo, et al., Nat. Mat.,12, 191-201 (2013) [2] G. L. W. Hart, et al., Phys. Rev. X 3, 041035 (2013) [3] P. Giannozzi, et al., J.Phys.:Condens.Matter, 21, 395502 (2009)

MM 42.3 Wed 12:45 BAR 205

High throughput modelling of novel borides — •David Holec[1], Vincent Moraes[2], Mirjam Arndt[3], Peter Polcik[4], and Paul Mayrhofer[5] — [1]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [2]Christian Doppler Laboratory for Application Oriented Coating Development at the Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [3]Oerlikon Balzers, Oerlikon Surface Solutions AG, Balzers, Liechtenstein — [4]Plansee Composite Materials GmbH, Lechbruck am See, Germany — [5]Institute of Materials Science and Technology, TU Wien, Vienna, Austria

Recently, computationally-driven understanding and exploring of materials have gained a lot of attention. One very prominent example of the fruitful symbiosis between theory and experiment is protective coatings based on nitrides. There, modelling serves as a reliable trend-giver and often provides also quantitative predictions.

In the quest of exploring new hard materials, we employ high-throughput *ab initio* modelling to transition metal borides, in order to characterise their structure, stability, and mechanical properties. The obtained trends are used for deciding on perspective systems (e.g., the Ti-W-B system) for further experimental validation and application-orientated coating development.

MM 42.4 Wed 13:00 BAR 205

Atom-mining: Improving the spatial resolution of Field Ion Microscopy using atomistic simulations and data mining — •Gh Ali Nematollahi[1], Shyam S. Katnagallu[1], Michal Dagan[2], Baptiste Gault[1], Blazej Grabowski[1], Paul Bagot[2], Michael Moody[2], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany — [2]Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH UK

Field Ion Microscopy (FIM) relies on the ionization of inert gas atoms from the specimen surface subjected to an intense electric field. Any FIM image represents a "snapshot" of individual surface atoms and 3D information of the bulk can be obtained by removing the surface atoms using field evaporation. However, the analysis of the atomistic information is not straightforward due to strong deformations and intensity variations caused by the electric field, and so far automated techniques to reconstruct the 3D atomistic structure are lacking. In this work, building on recent efforts by Dagan et al.[Microsc. Microanal.], we developed a new framework for automated reconstruction, using data mining and atomistic simulation techniques. In particular, different unsupervised and semi-supervised machine learning techniques are used to detect atoms, crystallographic planes and defects in FIM image. The results show that machine learning can be successfully employed to correct for the deformation of the sample caused by the strong electric fields. In a last step, atomistic relaxation based on empirical potentials is used to further improve the 3D-reconstructed data.

MM 43: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - hybrid and structured electrolytes

Time: Wednesday 11:45–12:45 Location: IFW A

MM 43.1 Wed 11:45 IFW A

Morphology and conductivity of nanohybrid block copolymer electrolyte for lithium-ion batteries — •Ezzeldin Metwalli, Maximilian Kaeppel, Simon Schaper, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Polymer electrolyte membranes are promising alternatives to conventional liquid electrolytes in lithium-ion batteries [1]. A key challenge is to achieve a highly ionic conductive solid-state polymer membrane that maintains high-modulus, toughness, and chemical stability. The ionic conductivity in relation to the morphology of a ternary system composed of polystyrene-block-polyethylene oxide (PS-b-PEO) diblock copolymer (DBC) electrolyte, lithium salt and ionic liquid (IL) was investigated. An optimized functional morphology of the hybrid membrane was achieved by enabling highly interpenetrated hard PS and soft PEO/IL domains. The high-modulus glassy PS domain of the nanostructured hybrid membranes offers mechanical stability, while the Li-containing PEO/IL hybrid domain enables the requisite high ionic conductivity. The IL doping enhances the solubilization of the undissociated lithium salt at the PS/PEO domain interface. The pronounced conductivity enhancement of the current Li-ion/IL/DBC hybrid electrolyte compared to other previously reported DBC electrolyte systems is discussed. [1] E. Metwalli et al., ChemPhysChem 2015, 16, 2882.

MM 43.2 Wed 12:00 IFW A

Preparation of Electrodes for Li-Ion Batteries from Inexpensive Dirty Silicon — •Richard Schalinski[1], Stefan L. Schweizer[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle 06099, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM, Halle 06120, Germany

With the increased development of renewable energies and electric vehicles in our society, there is a greater demand for high capacity, safe and inexpensive storage technologies. Li-ion batteries are the technology of choice for the use in portable devices. To increase the capacity density of these batteries, nanostructured silicon was introduced as a material for the negative electrode. Commonly, either expensive silane or electrical grade silicon is used as the starting material. We introduce an alternative route by using inexpensive metallurgical grade silicon (purity 98%) as a starting material and purify it using metal assisted chemical etching followed by ball milling to obtain silicon nanoparticles. The Si-nanoparticles where mixed with different binders (CMC, PVdF, Na-Alginate) to form slurries, which were coated onto Cu-substrates. The dried electrodes where investigated by SEM and introduced to further electrochemical testing in a half cell setup. A variation of the chemical contents and pretreatments of the substrates were carried out to optimize the capacity and cyclability of the electrodes.

MM 43.3 Wed 12:15 IFW A

Polymer paterning: Solid polymer electrolytes for lithium batteries — Preston Sutton, Ilja Gunkel, and •Ulli Steiner — Adolphe Merkle Institute, Fribourg, Switzerland

Patterning materials at the nanoscale can dramatically influence the performance of batteries. At the Adolphe Merkle Institute (AMI) we are applying expertise in structural control to improve electrodes and electrolytes alike. Two goals of our research are: 1- Take advantage of polymer self-assembly as a facile method to attain predictable morphologies in block copolymers (BCPs) quantifying ionic conductivity as a function of grain size and crystallinity. 2- Use BCPs to decouple mechanical properties from ionic conductivity in electrolytes.

MM 43.4 Wed 12:30 IFW A

Modulation of the optical properties of LiMn2O4 via Li-ion transport — •Yug Joshi, Susann Nowak, and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

Extensive research has been carried out in the fields of Li-ion batteries and electrochromic materials. The present study combines both in investigating the changes in the optical properties of the lithium manganese oxide (LMO), a spinel structured cathode material during an electrochemical reaction. To study this behaviors ion-beam sputtering is used to deposit LMO as the active layer onto a layer of platinum serving as a current collector, over an oxidized silicon wafer. The multilayered sample is then characterized using optical spectroscopy at different lithiation states. The measured data is fitted using Cauchy's model to extract the complex refractive index (refractive index and absorption coefficient) of LMO and its dependence on the lithium content. The reversibility of the optical changes is verified by in-situ optical measurements during multiple charging and dis-charging cycles of LMO. The study reveals a reversible change of the complex refractive index during an electrochemical reaction in the wavelength range of 850-1600nm, making it a suitable candidate for the application of optical switching.

MM 44: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Nano-porous materials

Time: Wednesday 11:30–13:15 Location: IFW B

Topical Talk MM 44.1 Wed 11:30 IFW B

Manipulating interfaces in nanoporous metals: Towards robust nanostructured materials with novel functionalities — •Nadiia Mameka — Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, 21502 Geesthacht, Germany

Nanoporous metals formed via dealloying emerge as a new class of nanomaterials in which high mechanical strength and stiffness can be successfully combined with diverse functional properties. The materials offer facile and controllable modification of their numerous internal interfaces through: *i)* tailoring size of their structural nanoscale constituents – nanoligaments – via thermal or electrochemical annealing, and *ii)* reversible altering of electronic and/or chemical structure of the nanoligaments by external stimuli.

The talk aims at demonstrating how imposing the consequences of both surface engineering approaches can be for actuation, strain sensing, and mechanical response of nanoporous metals with macroscopic dimensions. Here, the functionalities arise from electrocapillary coupling at the metal/fluid interface in hybrid composites made from nanoporous gold and aqueous electrolytes, where the control over the interface properties is realized by reversible changes of external control variables (surface charge density and/or adsorbate coverage) as the function of the electrode potential. The possibilities for further improvements of structural and functional properties in such hybrid nanomaterials will be also discussed.

MM 44.2 Wed 12:00 IFW B

Nanostructure Formation during Dealloying: Theory and Experiment — •Anastasia V. Strasser and Jörg Weissmüller — Hamburg University of Technology

From an empirical point of view, the corrosion conditions for making high quality nanoporous gold samples by dealloying silver-gold solid solutions are well established. The ligament size and the composition of the nanoporous material can be tuned in a reproducible way. Yet, the mechanisms and driving forces of the nanostructure formation are only partly understood. Our understanding of the process relies on the model by Erlebacher and co., that considers a balance between dissolution of the less noble element and surface diffusion of the more noble element, along with nucleation of corrosion on deeper terraces. From an experimental point of view, alloy corrosion has seen STM (scanning tunneling microscope) studies under conditions of passivation. Since bulk dealloying is achieved in the regime where the dissolution outruns the passivation, additional studies of that regime are of high interest. Here we present a direct atomic scale observation of the nanostructure formation during electro- chemical dealloying using in-situ EC-STM (electrochemical scanning tunneling microscope) in the bulk dealloying regime and the results from the corresponding kinetic Monte-Carlo simulation. Series of pictures showing subsequent steps of the structure formation can be correlated to the corrosion rate. Our results from in-situ STM observations and KMC simulation confirm essential suppositions of the current understanding.

MM 44.3 Wed 12:15 IFW B

Topological changes in coarsening networks — •Dana Zöllner[1] and Paulo R. Rios[2] — [1]Institute of Structural Physics, Technical University Dresden, Dresden, Germany — [2]Escola de Engenharia Industrial Metalúrgica, Universidade Federal Fluminense, Volta Redonda, Brasil

The topology of polygonal networks in materials like grain and foam microstructures has been a topic of scientific interest for decades - not only for mathematicians but also for materials scientists due to their imfortance for materials properties. Such networks consist in two dimensions of edges and vertices. As a result, a certain number of edges and likewise vertices surround a polygonal area, which forms a cell or grain.

In the present work, we show what kind of topological changes occur in such two-dimensional networks. To that aim, computer simulations of ideal coarsening have been carried out for different initial networks and at different coarsening stages. We will follow the temporal development of topological changes as well as the trajectories of individual cells.

MM 44.4 Wed 12:30 IFW B

Hierarchically structured nanomaterials — •Benedikt Roschning[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Porous microstructures used as functional materials often demand contradictory requirements on the pore size, which may be tackled by hierarchical structures consisting of porosity on different length scales. The aim of our project is the development of manufacturing routines for hierarchically structured nanomaterials combining different electrochemical approaches. Previous work focused on the preparation of nanoporous gold via corrosion of a dilute Au-Ag solid solution yielding a nanoporous Au-Ag alloy as intermediate product [1]. Coarsening creates the upper hierarchy level which can be corroded a second time to create the lower hierarchy level. However, corrosion induced shrinkage leads to intense crack formation making the material unsuitable for mechanical applications. Addition of Pt to the master alloy favors a high Au retention in the first dealloying step, reduces the shrinkage, prevents crack formation and allows the production of mm sized samples [2]. Yet, complete corrosion of the specimen and functionalization need to be shown.

[1] Qi, Weissmüller, ACS Nano 7 (2013) 5948-5954.

[2] Qi, Vainio, Kornowski, et al., Adv. Funct. Mater. 25 (2015) 2530-2536.

MM 44.5 Wed 12:45 IFW B

Bulk density measurements of small solids using Laser Confocal Microscopy — •Askar Kilmametov[1], Stefan Walheim[1], and Horst Hahn[1,2] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Technische Universität Darmstadt (TUD), Joint Research Laboratory Nanomaterials (KIT and TUD), Jovanka-Bontschits-Straße 2, Darmstadt 64287, Germany

A novel approach for precise density measurement of a small weight samples in the range of 1-3 mg is presented. A new kind of displacement method has been developed, by which a solid object is dropped into a semi-confined cylindrical cavity, which is filled with a nonvolatile liquid, to determine the volume of the sample. Due to surface tension, the upper level of the liquid forms a spherical meniscus pinned at the circular contact line, which is limited by a printed hydrophobic self-assembled monolayer. Monitoring of the liquid level is performed by confocal laser microscopy with a micrometer resolution. A straightforward procedure is developed to build-up a mass/volume linear dependence. This enables to determine the density of small solids with an accuracy of $<0.5\%$. The method appears to be very sensitive to open and closed porosity. Applying a vacuum of 20 mbar to the already immersed samples allows to perform quantitative porosimetry on a rather limited amount of material of only 0.25 microliter. This corresponds to about 2-5 mg for most metals, 1-2 mg for most ceramics, or even only 0.25-1 mg for organic materials.

MM 44.6 Wed 13:00 IFW B

Hierarchical Nanoporous Nickel as Bulk Electrochemical Actuators — •Chuan Cheng[1], Lukas Lührs[1], Tobias Krekeler[2], and Jörg Weissmüller[1] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Central Division of Electron Microscopy, Hamburg University of Technology, 21073 Hamburg, Germany

Materials which can mimic the properties of mammal muscles upon outside electrical/chemical triggering are called artificial muscles. Commercialized actuation materials such as piezoceramics, electroactive polymers and shape memory alloys are restricted by ultra-high actuation voltages, or small strain amplitude, or rather low energy efficiency. In the last decade, increasing attention has been paid to nanostructured materials, including nanoporous metals, carbon nanotubes, conducting polymers, nanographene, and so on, to transform electrochemical energy into mechanical energy for potential applications as artificial muscles. Nanoporous metals for artificial muscle applications have unique combination of low operating voltage, relatively high strain amplitude, high strength and stiffness compared with high voltage operated piezoceramics and soft polymer based actuators. We present a 3-D macroscopic actuator composed of nanoporous structured nickel with dual-scaled pores, in which the large sized pores facilitate fast ion transfer kinetics and small sized pores contributed to the large surface area for surface charge storage and strain generation. Advanced actuation performances with both high strain amplitude and strain rate were obtained.

MM 45: Invited talk Kargl

Time: Wednesday 15:00–15:30 Location: BAR 205

Invited Talk MM 45.1 Wed 15:00 BAR 205

Diffusion in liquid metals and alloys — •Florian Kargl — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, 51170 Köln, Germany

Chemical and self-diffusion coefficients of liquid metals and alloys are important input parameters for modelling of solidification, they serve as benchmark for refining molecular dynamics simulations, and they are intrinsically interesting for a better understanding of transport-property relations. Standard methods used for measuring diffusion coefficients are in a non-predictable way subject to external perturbations. This leads to a deviation from purely diffusive behaviour. The resulting effective diffusion coefficients can easily differ by up to 100% from their real value. In recent years, the accuracy in the experimental determination of diffusion coefficients was greatly enhanced by employing quasielastic neutron scattering to determine self-diffusion coefficients and by real-time monitoring of the chemical diffusion process employing X-ray radiography. At an uncertainty of less than 10% for the former and of about 20% for the latter, temperature dependencies and relations between different transport coefficients can be compared with theoretical predictions. Here, we show that: i) self-diffusion coefficients follow an Arrhenius-dependence around the melting point; ii) glass forming-systems show deviations from Stokes-Einstein behaviour; iii) the Darken relation has some shortcomings in predicting chemical diffusion coefficients. We finally highlight the importance of accurate values by comparing modelling results with real-time experiments for microstructure evolution.

MM 46: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V

Time: Wednesday 15:00–18:15 Location: GER 38

MM 46.1 Wed 15:00 GER 38

First-principle Linear Response in Real Space — •Honghui Shang[1], Danilo S. Brambila[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Density-functional perturbation theory (DFPT) has developed into an important computational tool for assessing the linear electronic response of crystalline solids to perturbations, e.g., from electric fields or nuclear displacements [1]. In this work we present a full real-space reformulation of DFPT and its implementation [2] in the all-electron, numeric atom-centered orbital electronic structure theory code FHI-aims. We discuss the specific contributions, e.g., relativistic effects and Pulay terms, that arise in such a formulation and validate our implementation by systematically comparing with the finite-difference approach for various extended systems. The computational efficiency is then analyzed via scaling and scalability tests on massively parallel architectures (CRAY and IBM x86 clusters). Finally, we show that this real-space formalism enables an arbitrarily dense sampling of the Brillouin zone by numerically cheap Fourier transformations, which in turn facilitates an efficient evaluation of the electron-phonon coupling matrix elements. We demonstrate the efficiency by computing the relaxation time of hot carriers in Si.

[1] X. Gonze and C. Lee, *Phys. Rev. B* **55**, 10355, (1997).
[2] H. Shang, *et al.*, *Comp. Phys. Comm. (accepted)*, arXiv:1610.03756.

MM 46.2 Wed 15:15 GER 38

Anharmonic Vibrations in Solids: Why and When Going Beyond Perturbative Treatments is Necessary — •Hagen-Henrik Kowalski, Maja-Olivia Lenz, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In *ab initio* theory, the nuclear motion is typically assessed using a truncated second order Taylor expansion for the potential energy (harmonic approximation). Recent computational and methodological advancements [1] allow to extend this expansion to the third order so to approximately treat also anharmonic effects. Little is known, however, about the role of higher order terms. In this contribution, we systematically compare how a third-order expansion performs with respect to techniques that are able to capture higher degrees of anharmonicity, e.g., the quasi-harmonic approximation and fully anharmonic molecular dynamics. For this purpose, anharmonic properties such as the thermal expansion and the Grüneisen parameters are computed for a set of materials with increasing degree of anharmonicity (Si, Mg_2Si, CuCl, and ZrO_2). This reveals that a third order expansion can still lead to quantitative and even qualitative errors at elevated temperatures and/or in highly anharmonic systems. Eventually, we discuss the impact of the chosen exchange-correlation functionals on these calculations and the implications of these findings for the computation of thermal conductivities [2].

[1] D. A. Broido, *et al.*, *Appl. Phys. Lett.* 91, 231922 (2007).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *ArXiv:* 1608.06917.

MM 46.3 Wed 15:30 GER 38

Anharmonic and Quantum Fluctuations in Molecular Crystals from Ab Initio Simulations — •Mariana Rossi[1] and Michele Ceriotti[2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Molecular crystals often exist in multiple competing polymorphs which are challenging to be predicted computationally, but show significantly different physicochemical properties. This challenge is not due only to the combinatorial search space, but also to the complex interplay of subtle effects determine the relative stability of different structures. Here we estimate all contributions to the free energies of these systems with density-functional theory, including the oft-neglected anharmonic contributions and nuclear quantum effects, by using a series of different flavors of thermodynamic integration. As an example, for the two most stable forms of paracetamol we find that anharmonic contributions, different descriptions of van der Waals interactions, and nuclear quantum effects **all** matter to quantitatively determine the stability of different phases [1]. Our studies indicate that anharmonic free energies could play an important role for molecular crystals composed by large molecules and opens the way for a systematic inclusion of these effects in order to obtain a predictive screening of structures. [1] Rossi, Gasparotto, Ceriotti, *PRL* **117**, 115702 (2016).

MM 46.4 Wed 15:45 GER 38

Exact solutions and approximations in the exact factorization of the electron-nuclear wavefunction — •Graeme Gossel and Neepa Maitra — Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065.

”Recently it was shown how a molecular wavefunction may be written exactly as a single product of a nuclear and an electronic wavefunction, with a pair of corresponding equations of motion [1]. This exact factorization provides a new and rigorous starting point for developing intuitive and physical approximations to the exact coupled system. Strikingly, in this factorized picture the electronic Hamiltonian is not strictly Hermitian. Nevertheless, the norm is conserved so long as certain terms persist. This, and other constraints, inform the approximations we apply to make the process numerically feasible. In parallel we present numerical self-consistent solutions of the exact factorization equations devoid of approximations to assess accuracy and behaviour of different terms. Finally, we discuss how a well characterized and robust single-product-picture such as this may be used in TDDFT calculations.

[1] A Abedi, NT Maitra, and EKU Gross, PRL 105 (12), 123002, 2010

MM 46.5 Wed 16:00 GER 38

Insight into time-propagation TDDFT excitations via Kohn–

Sham decomposition — •Tuomas P. Rossi[1], Mikael Kuisma[2,3], Martti J. Puska[1], Risto M. Nieminen[1], and Paul Erhart[2] — [1]Aalto University, Espoo, Finland — [2]Chalmers University of Technology, Gothenburg, Sweden — [3]University of Jyväskylä, Jyväskylä, Finland

The real-time-propagation formulation of time-dependent density-functional theory (RT-TDDFT) is an efficient method for calculating optical excitations of large molecules and nanoparticles. However, within RT-TDDFT, the analysis of the response is often limited to photoabsorption spectra and induced densities, in contrast to linear-response formulations of TDDFT, such as the Casida method, in which one can obtain further understanding on the basis of the Kohn–Sham electron-hole decomposition of the excitations.

In this work, we show that the Kohn–Sham decomposition can be equivalently obtained from RT-TDDFT calculations. We demonstrate the approach for the optical response of organic molecules and large metallic nanoparticles. The focus is especially on plasmonic applications, for which the method enables the analysis in terms of transition contribution maps [1]. By using the decomposition, we can shed light on the microscopic origin of plasmon resonances and their damping via plasmon–single-electron coupling, while retaining the favorable scaling of RT-TDDFT compared to linear-response formulations.
[1] S. Malola *et al.*, ACS Nano **7**, 10263 (2013).

MM 46.6 Wed 16:15 GER 38

Gauge-invariant Magnetic Properties from Time-Dependent Current-Density-Functional Theory — •Nathaniel Raimbault[1], Paul de Boeij[3], Pina Romaniello[2], and Arjan Berger[1] — [1]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier — [2]Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier — [3]University of Twente, Faculty of Science and Technology, Physics of Interfaces and Nanomaterials

Standard formulations of magnetic response properties are often plagued by gauge dependencies, which can lead to unphysical results, and to a slow convergence with basis-set size. In this talk we present a novel method for obtaining magnetic properties from the current density [1]. This alternative scheme is fully gauge-invariant, numerically efficient, and can be applied to any method from which the current density can be obtained. To illustrate our method, we applied it to time-dependent current-density-functional theory (TDCDFT). While different types of magnetic properties can be calculated in this way, we here emphasize the calculation of circular dichroism spectra, which are notably important in order to characterize secondary structures in biomolecules. The circular dichroism spectra we thus obtain for methyloxirane, dimethyloxirane and α-pinene are in good agreement with experiment [2]. [1] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, PRL 114, 066404 (2015); [2] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, JCTC 12, 3278 (2016)

MM 46.7 Wed 16:30 GER 38

Calculation of charge transfer integrals using constrained-DFT — •Tobias Lettmann and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Deutschland

For the investigation of charge transport properties of organic semiconductor materials, the fast and accurate calculation of charge transfer integrals (or transition matrix elements) is desirable. It has been suggested that the transfer integrals depend on a universal linear function of the corresponding wavefunction overlap, which can then be used to approximate the integral at a reduced computational cost[1].

We have calculated transfer integrals for dimers of poly(3-hexylthiophene) (P3HT) and diperylene bisimide (DiPBI), which are used in organic solar cells, in a large variety of intra- and intermolecular conformations and polymer lengths using a constrained-DFT approach[2]. Our results show, that there is indeed a universal relation between transfer integral and wavefunction overlap. However this relation is (i) nonlinear for large overlaps and (ii) only holds true if the transfer integral is rescaled by the number of electrons of the respective system.

[1] F. Gajdos et al.: *J. Chem. Theory Comput.*, 2014, **10**, 4653

[2] H. Oberhofer, J. Blumberger: *J. Chem. Phys.*, 2010, **133**, 244105

MM 46.8 Wed 16:45 GER 38

Towards ultra long-range ab-initio calculations — •Tristan Müller[1], Sangeeta Sharma[1,2], Eberhard K.U. Gross[1], and John K. Dewhurst[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [2]Department of physics, Indian Institute for Technology-Roorkee, 247997 Uttarkhand, India

We propose a generalization of the Bloch state which involves an additional sum over a finer grid in reciprocal space around each k-point. This allows for ab-initio calculations of ultra long-range modulations in the density which may involve millions of unit cells but with an efficiency rivaling that of a single unit cell. This is due to a new algorithm developed specifically for solving the particular eigenvalue problem that this ansatz requires. Thus physical effects on the micron length scale, which nevertheless depend on details of the electronic structure on nanometer length scales, can be computed exactly within density functional theory.

MM 46.9 Wed 17:00 GER 38

Local density fitting within a Gaussian and plane waves scheme for large-scale density functional theory calculations — •Dorothea Golze[1,2], Marcella Iannuzzi[1], and Jürg Hutter[1] — [1]Aalto University, Otakaari 1, 02150 Espoo, Finland — [2]University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

A local resolution-of-identity (LRI) approach is introduced in the Gaussian and plane waves (GPW) scheme to enable large-scale Kohn-Sham (KS) density functional theory calculations. The construction of the KS matrix in GPW scales already linearly with respect to system size by using a plane wave expansion of the density for the evaluation of the Coulomb term in combination with a local basis. The intention is to retain the linear scaling of the GPW approach, while reducing the prefactor for computing the KS matrix. The locality of the density fitting ensures an $O(N)$ scaling and is implemented by approximating the atomic pair density by an expansion in one-center fit functions. The prefactor is smaller with LRI since the computational demands for the grid-based operations become negligible, while they are dominant in GPW. We observe a speed-up of the self-consistent field (SCF) procedure by a factor of up to 30 for periodic systems dependent on the symmetry of the simulation cell and the grid cutoff. The accuracy of LRIGPW is assessed for different systems and properties. Generally, total energies, reaction energies, intramolecular and intermolecular structure parameters are well reproduced. LRIGPW yields also high quality results for extended condensed phase systems such as liquid water, ice XV and molecular crystals.

MM 46.10 Wed 17:15 GER 38

From the Electron Localization Function to a Coalescent-Pair Locator — •Stefano Pittalis[1], Daniele Varsano[1], Alain Delgado[2,3], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze, Consiglio Nazionale dellle Ricerche, Via Campi 213a, 41125 Modena, Italy — [2]Department of Physics, University of Ottawa, Ottawa, ON K1N 6N5, Canada — [3]Centro de Aplicaciones Tecnológicas y Desarrollo Nuclear, Calle 30 # 502, 11300 La Habana, Cuba

The Electron Localization Function (ELF), as proposed originally by Becke and Edgecombe, uses the information on the distribution of pairs of electrons with parallel spins. The ELF has been widely adopted as a descriptor of atomic shells and covalent bonds, but it is not useful to visualize the bond in H_2 – the simplest neutral molecule in the universe. Here we propose a complementary descriptor which also works for H_2 by exploiting the information on pairs of electrons with opposite spins. Remarkably, only quantities derived from occupied single-particle orbitals are required in the calculations. If time allows, implications for developing improved approximate density functionals will also be discussed.

MM 46.11 Wed 17:30 GER 38

Band structure interpolation via maximally localized Wannier functions implemented in LAPW+lo basis — •Sebastian Tillack, Andris Gulans, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

The band structure is one of the most fundamental quantities of any solid that carries a lot of information about the material's properties. Obtaining a smooth dispersion from density-functional theory (DFT) and especially from the *GW* approximation of many-body perturbation theory may be very expensive. To this extent, we have implemented a method for generating maximally localized Wannier functions (WF) [1] from Kohn-Sham wavefunctions in the full-potential all-electron code `exciting` [2] using a (linearized) augmented plane-waves plus local-orbitals basis. These WF are used for interpolating wavefunctions and corresponding eigenenergies for arbitrary **k**-points in a computationally cheap post-processing step. The interpolated Kohn-Sham and *GW* bands of conventional and two-dimensional semiconductors and insulators are also used as an input to calculations of optical-excitation spectra.

[1] N. Marzari and D. Vanderbilt, *Phys. Rev. B* ***56***, 12847 (1997)
[2] A. Gulans, et al. *J. Phys.: Condens. Matter* ***26***, 363202 (2014)

MM 46.12 Wed 17:45 GER 38

Chemical insight from Fermi-Löwdin orbitals — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore Maryland (MD), US

The recently developed Fermi-Löwdin orbital based method for correcting the self-interaction error in Density Functional Theory (FLO-SIC DFT) [1,2,3] is briefly introduced. Contrary to standard DFT approaches, where only auxiliary Kohn-Sham orbitals are available, FLO-SIC DFT delivers a set of well-defined, localised Fermi-Löwdin orbitals. These localised orbitals together with their optimised reference positions yield an inherently 'chemical' representation of bonding details in molecules that resembles remarkably well Lewis concept of lone and binding electron pairs. For complex examples, the method provides detailed insights into the bonding situation in terms of multicenter many-electron bonds in a natural, chemically-intuitive fashion.

[1] M. R. Pederson et al., JCP 140, 121103 (2014).
[2] M. R. Pederson, JCP 142, 064112 (2015).
[3] T. Hahn et al., JCP 143, 224104 (2015).

MM 46.13 Wed 18:00 GER 38

Conditions for describing triplet states in reduced density matrix functional theory — Iris Theophilou[1], Nektarios N. Lathiotakis[2], and •Nicole Helbig[3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

We consider necessary conditions for the one body-reduced density matrix (1RDM) to correspond to a triplet wave-function of a two electron system. The conditions concern the occupation numbers and are different for the high spin projections, $S_z = \pm 1$, and the $S_z = 0$ projection. Hence, they can be used to test if an approximate 1RDM functional yields the same energies for both projections. We employ these conditions in reduced density matrix functional theory calculations for the triplet excitations of two electron systems. In addition, we propose that these conditions can be used in the calculation of triplet states of systems with more than two electrons by restricting the active space. We assess this procedure in calculations for a few atomic and molecular systems. We show that the quality of the optimal 1RDMs improves by applying the conditions in all the cases we studied.

MM 47: Topical session: Data driven materials design - ab initio materials design

Time: Wednesday 15:45–17:00 Location: BAR 205

Topical Talk MM 47.1 Wed 15:45 BAR 205

Finite-temperature simulations of materials properties for data-driven materials design — •Igor Abrikosov — Linköping University, Linköping, Sweden — National University of Science and Technology MISIS, Moscow 119040, Russia

A systematic knowledge-based search for new materials using data-driven approaches combined with the electronic structure theory is now established as a recognized field within condensed matter physics and materials science. We show that by means of computer experiments it is possible to obtain relevant materials parameters which are difficult, expensive or impossible to obtain in physical experiments. With these tools at hands, theory is capable to guide experimental synthesis of new materials [1] as well as discoveries of exciting phenomena with high potential for novel technologies [2]. We present new approaches that allow to bring simulations conditions much closer to those at which materials operate in tools and devices. In particular, we focus on simulations at finite temperatures and discuss the results obtained for transition metal alloys [3] as well as for transition metal nitrides [4]. We argue that using novel tools increases reliability of theory underlying data-driven materials design.

[1] A. S. Ingason, et al., Phys. Rev. Lett. 110, 195502 (2013). [2] V. Ivády, et al., Phys. Rev. Lett. 117, 220503 (2016). [3] M. P. Belov, N. V. Skripnjak, A. V. Khvan, A. Dinsdale and I. A. Abrikosov, in preparation. [4] N. Shulumba, et al., Phys. Rev. Lett. 117, 205502 (2016).

MM 47.2 Wed 16:15 BAR 205

Evolution of defect populations in silicon carbide : coupling ab initio energetics, charged defects and rate theory — •Guido Roma, Thomas Jourdan, Quentin Bouton, Jean-Paul Crocombette, and Fabien Bruneval — DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif sur Yvette, France

Ab initio based evolution of defect populations using stochastic methods or rate theory has been developed since at least a decade and has provided the explanation of the evolution of material properties of irradiated materials [1]. Its application concerns, however, mostly metals. Although applications to semiconductors or insulators exist [2], they overlook in most cases the variety of charge states of point defects. We discuss here an approach to overcome this limitation in the case of silicon carbide, where we dispose of a relatively complete database of defect energetics. We present some results of rate theory simulations for silicon carbide where intrinsic defects are supersaturated, as it happens for example under or after electron irradiation. In particular, we show examples where the mutual influence of doping and kinetics in the material matters, and we revisit our previous prediction of SiC nanodecomposition driven by vacancy-interstitial recombinations [3], where electrostatic effects were neglected. We discuss also the possibility of coupling this approach with the simulation of spectral properties, with the example of Raman spectra.

MM 47.3 Wed 16:30 BAR 205

Optical properties of disordered graphene quantum dots — •Abdulmenaf Altintas, Korhan Çakmak, and Alev Devrim Güçlü — Department of Physics, Izmir Institute of Technology, IZTECH, TR35430, Izmir, Turkey

We investigate the effects of disorder and electron-electron interactions on the optical properties of graphene quantum dots using tight-binding, mean-field Hubbard and configuration interaction approaches. We consider hexagonal armchair quantum dots containing up to 10806 atoms, where the disorder is modelled as a long-range random potential landscape, giving rise to electron-hole puddles. We show that disorder induced electron and hole localizations near Fermi level is reduced due to electron-electron interactions, making the observation of universal optical conductance robust against imperfections. When disorder is present, calculated absorption spectrum approaches the experimental results for isolated mono layer of graphene sheet.

MM 47.4 Wed 16:45 BAR 205

First-principles insight into the martensitic transformation and diffusion properties in Ti-Ta alloys — •Tanmoy Chakraborty, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44780 Bochum, Germany

In Ti-Ta-based high-temperature shape memory alloys (HTSMAs) the martensitic transformation temperature (M_s) exhibits a strong dependence on the chemical composition. A detailed knowledge of the underlying mechanisms and phase stability of the competing austenite and martensite phases in these alloys can aid the design of new HTSMAs with the desired functional properties at elevated temperatures. Using density functional theory in combination with the quasi-harmonic Debye model we approximate the different contributions to the free energy as a function of composition and compare the stability of competing phases at finite temperature. We identify the physical key parameters governing the experimentally observed composition dependence: the

0K energy difference and the difference in the Debye temperature between the involved phases. From our calculations we propose a one dimensional descriptor for high-throughput screening of M_s for the design of new HTSMAs. In addition to the thermodynamic phase stability we investigate the mobility of the different elements within the alloy as a function of composition and local environments which is key to analyze segregation and redistribution at elevated temperatures.

MM 48: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses III - plasticity and hetererogeneities

Time: Wednesday 15:45–17:15 Location: IFW A

Topical Talk MM 48.1 Wed 15:45 IFW A

Plastic deformation in amorphous solids: The role of elasticity and spatio-temporal correlations of fluctuations — •Fathollah Varnik and Muhammad Hassani — ICAMS, Ruhr-Universität Bochum, Germany

In view of their broad range of application, deformation behavior amorphous solids is of great practical and theoretical interest. Early experiments on bubble rafts and computer simulations of model glasses has revealed that particles rearrange collectively to accommodate for the globally imposed deformation/stress. Typically, these "shear transformation events" occur within small domains with a linear size of a few particle diameters. Mesoscopic elasto-plastic models highlight the role of system spanning elastic propagators for localized plastic deformation and shear banding. Recent experiments and simulations of hard sphere glasses underline the possible role of anisotropic correlations of plastic activity for shear banding. Microscopic theories, on the other hand, emphasize the role of local structure for the response to an externally imposed shear or stress. In this talk, we review these ideas, with a special emphasize on spatio-temporal correlations of plastic activity and its possible role for shear localization. The role of the fluctuations of the local structure, local forces and correlations thereof is also highlighted.

We are grateful to G. Wilde and S. Divinski for useful discussions. M.H. is partially supported by the Max-Planck Society. Computation time by the Jülich supercomputing center within the ESMI-programme (project No ESMI 17) is acknowledged.

MM 48.2 Wed 16:15 IFW A

Local mechanical properties of ultrastable metallic glass — •Thomas Dziuba, Yuansu Luo, and Konrad Samwer — I. Phys. Intitut, Univ. Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The recent discovery of so called ultrastable metallic glasses led to great opportunities for experimental examinations which may not only give insight to the physical properties of such glasses but also to the glass-forming process in general [1]. In this context, the talk will give an overview on our experimental work using vapor deposition to create different ultrastable CuZr-glasses. Especially the use of Atomic-Force-Acoustic-Microscopy (AFAM) makes the measurement of elastic properties on a nanometer-scale possible. Comparisons with ordinary glassy systems and crystalline material reveal the energetic state during the formation of the solid and line up perfectly with theoretical considerations and simulations. Therefore, information about the behavior of systems in the context of the potential energy landscape (PEL) could be derived and will be presented. Also, the influence of temperature and deposition rates on the formation of different phases in the solid was evaluated by using XRD-techniques. Here the goal is not only to understand the nature of ultrastable metallic glasses but additionally to gain the ability to tune such materials for optimal mechanical properties.

Acknowledgement: DFG-FG 1394 PI

[1] H. B. Yu, Y. Luo and K. Samwer: Ultrastable Metallic Glass. In: Adv. Mater. 25, 5904-5908 (2013)

MM 48.3 Wed 16:30 IFW A

Interface controlled plasticity in metallic crystal-glass composites — Constanze Kalcher, Tobias Brink, Omar Adjaoud, and •Karsten Albe — Technische Universität Darmstadt, FB 11, FG Materialmodellierung, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

The mechanical properties of metallic glasses can be modified by secondary phases. In the current contribution we study how the creep and deformation behavior of a metallic glass is altered by the presence of secondary crystalline and glassy phases. By means of molecular dynamics simulations, we show that not only the mechanical properties of the phase fractions but also interfaces affect the mechanical response of a Cu-Zr glass composite. We study various topologies and phase fractions and propose an explanation in terms of interface orientations and a resulting Schmid-like law. We finally show that it is possible to enhance the mechanical properties of nanoglasses by reinforcing their glassy interfaces.

MM 48.4 Wed 16:45 IFW A

Deformation and relaxation of AlYFe metallic glass ribbons — •Marius Gerlitz, Rene Hubek, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Metallic glasses and their deformation behavior are in the focus of current research. Plastic deformation of amorphous structures causes localized shear zones, so called shear bands. However, it is not fully understood to which extend the matrix carries deformation and alters its characteristics upon plastic deformation. Inherent thermal vibrations of atoms are sensitive to their mechanical coupling, thus, specific heat measurements at low temperatures are an excellent tool to analyze fundamental properties of vibrational modes. In the present work, an AlYFe glass was chosen as a model system to analyze the influence of deformation on excess contributions to the specific heat at low temperatures, known as Boson peak. Specimen-states were examined including heat capacity measurements via a 2-Tau-Method subsequent to characterization through x-ray-diffraction and calorimetric measurements. Results are discussed in comparison to the available literature on the Boson peak of metallic glasses. Specifically it was found that the relaxation behavior of metallic glasses is enhanced by the presence of shear bands. Due to the limited volume of shear bands, it is concluded that the mostly undeformed matrix additionally contributes to the relaxation.

MM 48.5 Wed 17:00 IFW A

Micro-alloying of Gd to a PdNiP-based bulk metallic glass — •Christian Buchholz, Niklas Nollmann, Harald Rösner, and Gerhard Wilde — Institut für Materialphysik, WWU Münster, Münster, Deutschland

Bulk metallic glasses (BMGs) are well known for their high hardness but also to exhibit almost no ductility when reaching the end of the elastic deformation range. It has been recently shown [N. Nollmann et al., Scripta Mater. (2015), http://dx.doi.org/10.1016/j.scriptamat.2015.08.030] that micro-alloying applied to $Pd_{40}Ni_{40}P_{20}$ by adding small amounts of Co or Fe (around 1 at%) can strongly improve or worsen the mechanical properties. Here we present new results obtained after adding Gd to $Pd_{40}Ni_{40}P_{20}$. Similar to Co, Gd also enhances the ductility of the produced BMG. However, the phase transformation from the undercooled liquid to the crystalline state is also strongly affected by the Gd addition, resulting in a highly unusual crystallization kinetics. The results and consequences are discussed.

MM 49: Microstructure and Phase Transformations - shape memory alloys

Time: Wednesday 15:45–16:45 Location: IFW B

MM 49.1 Wed 15:45 IFW B

Role of nano-precipitates in thermoelastic martensitic transformation in Fe-Mn-Al-Ni shape memory alloys — •Toshihiro Omori[1], Makoto Nagasako[2], and Ryosuke Kainuma[1] — [1]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan — [2]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Fe-Mn-Al-Ni alloy shows superelasticity associated with the α(bcc)/γ(fcc) martensitic transformation. Although Fe-Mn-Al ternary alloys show non-thermoelastic martensitic transformation, the addition of Ni results in the precipitation of fine β-NiAl (B2) particles and changes the transformation manner to thermoelastic. Therefore, it is considered that Ni plays a key role in the thermoelastic transformation. In this study, the effect of Ni on the martensitic transformation was investigated. The microstructures of Fe-36Mn-15Al-Ni (at%) alloys with different Ni contents were observed using TEM and HAADF-STEM. It was found that the β particle with about 10 nm is coherent with the martensite phase in 7.5Ni alloy, and the B2 lattice was distorted. In the martensite phase, the nano-twins were frequently introduced and the shear angle became smaller. These facts suggest that there is interaction between the β precipitate and martensite matrix due to the coherency, and it is deduced that the compatibility between the parent and martensite phases becomes high. The thermoelasticity comes from this microstructural feature.

MM 49.2 Wed 16:00 IFW B

Ordering Nanotwins in Modulated Martensite — Markus E. Gruner[1,2], Robert Niemann[2], Peter Entel[1], Rossitza Pentcheva[1], Ulrich K. Rössler[2], Kornelius Nielsch[2], and •Sebastian Fähler[2] — [1]Theoretical Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Modulated ferromagnetic martensites exhibit outstanding magnetocaloric and magnetic shape memory properties. Focusing on the Ni2MnGa prototype system, we use large scale density functional theory calculations to demonstrate that the formation of modulated martensite and key functional properties are governed by ordering nanotwins. Ordering is driven by the interaction between twin boundaries, which oscillates with the distance between twin boundaries. Minimizing the interaction energy results in the experimentally observed ordered modulations at the atomic scale, it explains a particular type of stacking fault at the mesoscale, known as a/b twin boundaries, and contributes substantially to the macroscopic hysteresis losses. Furthermore, an analysis of the relaxation process reveals that phonon softening paves the way for the transition towards the nanotwinned martensite, which unifies both competing concepts to explain modulated martensite.

MM 49.3 Wed 16:15 IFW B

Impact of doping on the magnetic and structural transformations in magnetocaloric materials — •Biswanath Dutta, Vijaya Begum, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Understanding the magnetic and the martensitic transformations together with their coupling in magnetocaloric materials (MCMs) is crucial to tailor and optimize them for magnetic refrigeration. Specifically, any application of the MCMs requires a detailed knowledge of their underlying phase transformations. Within this study, we employ density functional theory along with Monte Carlo (MC) simulations to understand the impact of substitutional elements on the phase stability and the transformation behavior in Ni-Mn-based Heusler alloys. Our calculations reveal a reduction in the martensitic transformation temperature accompanied by a metamagnetic transition leading to a large entropy change due to Co substitution. We discuss the results in terms of calculated free energies, magnetic exchange interactions and the magnetic moments. The coupling of the magnetic and the structural degrees of freedom and its influence on the transformation behavior is addressed using MC simulations with the DFT input. Based on the achieved results, we provide new insights into the effect of doping on the martensitic and the magnetic transformations in Heusler alloys.

MM 49.4 Wed 16:30 IFW B

Vacancy annihilation and ordering kinetics in Ni_2MnAl studied by PALS — •Georg Zagler[1], Pascal Neibecker[1,2], Michael Leitner[1,2], Josef Schmidbauer[1,2], and Christoph Hugenschmidt[1,2] — [1]Physik Department, Technische Universität München, 85747 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Heusler alloys are ternary intermetallic compounds with sum formula X_2YZ. These systems are of special interest due to them displaying the ferromagnetic shape memory effect (FSME) with strains larger than those of conventional actuators. While the protoypical ferromagnetic shape memory alloy Ni_2MnGa exhibits a martensitic transition and hence a pronounced FSME, the closely related Ni_2MnAl-System does not show this effect. Presumably this is due to a lack of atomic $L2_1$ order in the Ni_2MnAl system. Responsible for the reduced degree of order are the slow ordering kinetics in the temperature region of interest. Indirect measurements show that the achievable state of order in this system can however be influenced by quenched-in vacancies. A direct method to study vacancy concentrations in solids is positron annihilation lifetime spectroscopy (PALS). In the outlined work, we investigate the effect of quenched-in vacancies on the ordering kinetics of an off-stoichiometric Ni_2MnAl-alloy by means of PALS. We show a clear reduction of the average positron lifetime with the annealing time in isothermal annealing studies and correlate vacancy concentrations to ordering kinetics as determined by calorimetric measurements.

MM 50: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Structure - property relationships II

Time: Wednesday 15:45–16:45 Location: IFW D

MM 50.1 Wed 15:45 IFW D

Process monitoring of charging/discharging of lithium ion battery cathodes by operando SQUID magnetometry — •Roland Würschum[1], Gregor Klinser[1], Stefan Topolovec[1], Harald Kren[2], Stefan Koller[2], Walter Goessler[3], and Heinz Krenn[4] — [1]Inst. of Mater. Phys., Graz Univ. of Technology, Graz, Austria — [2]VARTA Micro Innovation GmbH, Graz — [3]Inst. of Chem., Univ. Graz — [4]Inst. of Phys., Univ. Graz

The magnetic susceptibility χ of cathode materials, which contain transition metals, substantially changes during charging/discharging and, therefore, serves as highly sensitive fingerprint for the charge state. A novel pathway in this direction has recently opened up by developing in-situ electrochemical techniques for magnetometry. Operando magnetic χ-measurements on Li_xCoO_2 [1] and $Li_xNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC) cathode materials [2] in a SQUID magnetometer during repetitive electrochemical cycling were performed enabling a continuous and bulk sensitive monitoring of the charge compensation process. Upon charging of NMC up to Li contents of $x = 1/3$ exclusively Ni undergoes oxidation, namely in two consecutive steps $Ni^{2+} \rightarrow Ni^{3+}$ for $x > 2/3$ and $Ni^{3+} \rightarrow Ni^{4+}$ for $2/3 > x > 1/3$ [2]. Co oxidation for $x < 1/3$ is found to be irreversible [2]. In the case of Li_xCoO_2, evidence is found for a nonmetal−metal transition of Anderson−type [1]. In addition to Co also O undergoes partial oxidation, as also observed for NMC.

[1] St. Topolevec et al., J. Sol. State Electrochem. 20 (2016) 1491.

[2] G. Klinser et al., Appl. Phys. Letters 109 (2016) 213901.

MM 50.2 Wed 16:00 IFW D

Enhancement of Sodium Ion Battery Performance Enabled

by Oxygen Vacancies — •Yang Xu, Min Zhou, Chengliang Wang, Liying Liang, Fabian Grote, Yan Mi, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

The utilization of oxygen vacancies (OVs) in sodium ion batteries (SIBs) is expected to enhance performance, yet it has rarely been reported. Taking the MoO3-x nanosheet anode as an example, for the first time we demonstrate the benefits of OVs on SIB performance. Moreover, the benefits at deep-discharge conditions can be further promoted by an ultrathin Al2O3 coating. Ex-situ electrochemical impedance and X-ray photoelectron spectroscopy measurements show that the OVs increase the electric conductivity and Na-ion diffusion coefficient, and the promotion from ultrathin coating lies in the effective reduction of cycling-induced solid-electrolyte interphase. The coated nanosheets exhibited high reversible capacity and great rate capability with the capacities of 283.9 mAh g-1 at 50 mA g-1 and 179.3 mAh g-1 at 1 A g-1 after 100 cycles. This work could not only arouse future attention on OVs for sodium energy storage, but also open up new possibilities for designing strategies to utilize defects in other energy storage systems.

Reference

Y. Xu, M. Zhou, X. Wang, C. Wang, L. Liang, F. Grote, M. Wu, Y. Mi, Y. Lei, Angew. Chem. Int. Ed. 2015, 54, 8768.

MM 50.3 Wed 16:15 IFW D

Polycrystalline NaxCoO2 thin films on ß-Alumina ceramics for solid state batteries — •Philipp Kehne[1], Conrad Guhl[2], René Hausbrand[2], and Philipp Komissinskiy[1] — [1]Department of Materials Science, TU-Darmstadt, Advanced thin film technology — [2]Department of Materials Science, TU-Darmstadt, Surface science

Good cycling performance was previously shown for rechargeable sodium ion batteries with layered-oxide cathode materials such as NaxCoO2 in combination with liquid electrolytes. However, studies of sodium-based solid state batteries are necessary to correlate the electronic structure of sodium-ion insertion materials with the battery performance. Here we report polycrystalline NaxCoO2 films grown on ß-Alumina polycrystalline ceramic substrates with pulsed laser deposition. The sodium content in the films can be adjusted in the range of x = 0.6 * 1.1 by varying the post-deposition annealing conditions. The ß-alumina substrates reveal ionic conductivities of 0.002 S/cm (25 °C) and can be used as electrolyte in solid-state sodium batteries. The fabricated Swagelok-type rechargeable batteries with NaxCoO2 thin-film cathodes, ß-alumina electrolyte, and sodium anodes reveal an open circuit voltage of 2.75 V and a specific capacitance of C = 80 mAh/g. Investigations of the electronic structure of the materials and interfaces in the fabricated batteries by in-situ XPS are in progress.

MM 50.4 Wed 16:30 IFW D

Large-scale highly ordered Sb nanorod arrays anode with high capacity and rate capability for sodium-ion batteries — •Liying Liang, Yang Xu, Chengliang Wang, Liaoyong Wen, Yaoguo Fang, Yan Mi, Min Zhou, Huaping Zhao, and Yong Lei — Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany.

The poor electrochemical performance of Na-ion batteries is the major bottleneck for future development. Hence a performance-oriented electrode structure is proposed, which is 1D nanostructure arrays with large-scale high ordering, well vertical alignment, and large interval spacing. Benefiting from these structure merits, a great enhancement on electrochemical performance could be achieved. To Sb as an example, we firstly report large-scale highly ordered Sb nanorod arrays with uniform large interval spacing (190 nm). In return for this electrode design, high ion accessibility, fast electron transport, and strong electrode integrity are presented here. Used as additive-free anode for SIBs, Sb nanorod arrays showed a high capacity of 620 mAh g-1 at the 100th cycle with a retention of 84% up to 250 cycles at 0.2 A g-1, and superior rate capability for delivering reversible capacities of 579.7 and 557.7 mAh g-1 at 10 and 20 A g-1, respectively. A full cell coupled by P2-Na2/3Ni1/3Mn2/3O2 cathode and Sb nanorod arrays anode was also conducted, which showed a good cycle performance up to 250 cycles, high rate capability up to 20 A g-1, and large energy density up to 130 Wh kg-1.

MM 51: Topical session: Data driven materials design - databases

Time: Wednesday 17:15–18:00 Location: BAR 205

MM 51.1 Wed 17:15 BAR 205

The NOMAD (Novel Materials Discovery) Laboratory: Concepts, Challenges, and Results [⋆] — •Pasquale Pavone[1], Georg Huhs[1,3], Luca Ghiringhelli[2], Claudia Draxl[1,2], and Matthias Scheffler[2] — [1]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany — [2]Fritz-Haber-Institut der MPG, Berlin, Germany — [3]Barcelona Supercomputing Center, Spain

The NOMAD (Novel Materials Discovery) Laboratory Center of Excellence (CoE), https://NOMAD-CoE.eu, is a community-driven activity with the mission to serve the whole field of materials science and engineering. It tackles the issues of Big Data in materials science, starting from the NoMaD Repository [1], which by now contains results from more than 18 million DFT total-energy calculations. This corresponds to several billion CPU-core hours spent on high-performance computers worldwide. With these and more and more incoming data, we build a Materials Encyclopedia, to provide a user-friendly access to all these results, also making use of Advanced Graphics. Novel Big-Data Analytics tools are developed for finding trends, identifying outliers, and predicting new materials with tailored properties. Thus, this talk describes the basic concepts and goals of the NOMAD CoE in order to stimulate a discussion and suggestions on how to proceed further. This work received funding from "The Novel Materials Discovery (NOMAD) Laboratory", a European Center of Excellence.

[⋆] Collaboration with the entire NOMAD team: https://nomad-coe.eu
[1] https://NOMAD-Repository.eu

MM 51.2 Wed 17:30 BAR 205

The NOMAD Analytics Toolkit: Interactive Big-Data Driven Materials Science over the Web — •Luca M. Ghiringhelli, Fawzi Mohamed, Ankit Kariryaa, Angelo Ziletti, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany [‡]

Big-data analytics opens new routes towards scientific insight by offering analysis tools that can reveal patterns, trends, and causal relationships so-far hidden in the data. The Novel Materials Discovery (NOMAD) Repository (`https://nomad-repository.eu`) stores millions of open-access materials-science calculations obtained with dozens of different codes. In order to perform analytics on this data, two further steps are necessary: i) the raw, code-specific inputs/outputs of the calculations need to be converted into a standardized format that uses one convention for, e.g., units, zero base lines, and file formats. We present a flexible and extensible metadata infrastructure (`https://metainfo.nomad-coe.eu`), implemented for storing the data in an intuitive, code-independent, representation. ii) the data needs to be easily and publicly searchable, retrievable, and analyzable. With the NOMAD analytics toolkit (`https://analytics-toolkit.nomad-coe.eu/`), we present an interactive web-interface that allows everybody, without need to install any software, to query and analyze the data. We demonstrate the toolkit with an analysis of oxide semiconductors data, looking for a structure-property relationship with statistical methods.

[‡] Collaboration with the full NOMAD team: `https://nomad-coe.eu`.

MM 51.3 Wed 17:45 BAR 205

The NOMAD Repository - a key service for the computational-materials science community — •Jungho Shin[1,2], Thomas Zastrow[3], Lorenzo Pardini[1], Stefan Heinzel[3], Matthias Scheffler[2], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany — [2]Fritz-Haber-Institut der MPG, Berlin, Germany — [3]Max Planck Computing and Data Facility, Garching, Germany

The NoMaD Repository, http://nomad-repository.eu/, is a community effort, offering to store and share input and output files of all popular electronic-structure codes. The uploaded files are saved for at least 10 years. Thus, uploaders and their groups can get back what they have done in the past, and also others can use the data for their own scientific work. The NoMaD Repository offers DOIs free of charge which makes the scientific data are citable. It is the only repository in materials science recommended by Nature Scientific Data. Currently, the NoMaD Repository contains more than 3 million entries, which corresponds to more than 18 million total-energy calculations and several billion CPU core hours spent on various high-performance computers worldwide. Recently, the open-access data have been parsed and normalized by the NOMAD Laboratory, https://nomad-coe.eu/. Its Archive contains normalized, (largely) code-independent data, which is an important prerequisite for data-driven materials science. This work received funding from "The Novel Materials Discovery (NOMAD) Laboratory", a European Center of Excellence.

(**) Collaboration with the entire team: http://nomad-repository.eu

MM 52: Microstructure and Phase Transformations - phase stability

Time: Wednesday 17:00–18:00 Location: IFW B

MM 52.1 Wed 17:00 IFW B

Microstructure-engineering of near-α titanium alloys — •Stefanie Sandlöbes[1,2], Zahra Tarzimoghadam[2], Sandra Korte-Kerzel[1], and Dierk Raabe[2] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Lean alloying of the beta-stabilizing elements Fe and Mo to titanium in combination with appropriate heat treatments enables one to manipulate the microstructure. Consequently, the mechanical properties can be tailored covering a broad range from low yield strength and high ductility to high yield strength and medium ductility. By applying multi-scale characterization of the mechanical properties and microstructures it is shown that local segregation and partitioning phenomena on the nano-scale are causing local allotropic and martensitic transformations and significantly alter the active deformation mechanisms.

MM 52.2 Wed 17:15 IFW B

The applicability of grain boundary engineering on ultrafine grained Cu-Ni alloys — •Friederike Emeis, Martin Peterlechner, Harald Rösner, Sergiy V. Divinski, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, D-48149

Grain boundary engineering (GBE) is a concept used to design a thermal stable microstructure by the introduction of special grain boundaries ($\Sigma3$-, $\Sigma9$-GBs) and their conjunctions. Due to the poor thermal stability of severely deformed materials, GBE is of interest to design an ultrafine grained and thermally stable microstructure with retained enhanced properties. In the present investigation, GBE is applied to severely deformed Cu-Ni alloys (including the pure endmembers). Copper and nickel are completely miscible in the liquid and the solid state and thus the stacking fault energy (SFE) of the solid solutions also varies strongly and systematically for the different alloy compositions. The SFE is related to the tendency to undergo twinning ($\Sigma3$-GB). The annealing-induced microstructure evolution of the severely deformed Cu-Ni alloys is analyzed. Most of the concepts describing the microstructural behavior are only valid for pure materials. For the alloys, the concurrent effects from SFE and solid solution need to be considered. The data on the development of the GB structure and grain size lead to the conclusion that not only a small SFE but a second mechanism is important to prevent grain growth and to achieve a high fraction of suitable GBs. For Cu50Ni50 and Cu65Ni35 the microstructure was optimized.

MM 52.3 Wed 17:30 IFW B

Linear complexions - local phase transformation of dislocations — Alisson Kwiatkowski da Silva[1], Margarita Kuzmina[1], Dirk Ponge[1], Michael Herbig[1], •Stefanie Sandlöbes[1,2], Baptiste Gault[1], Sandra Korte-Kerzel[2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany

Complexions are confined interface-stabilized states which differ in structure and/or composition from the bulk. They form in many ceramic materials as 2D complexions. We use correlative transmission electron microscopy / atom probe tomography to show the existence of 1D complexions in a martensitic Fe9wt%Mn alloy. Equilibrium segregation of Mn to dislocations causes transformation of dislocation cores into austenite. These austenite regions are found to be confined to the strain field of the dislocation and remain sub-critical in size even after extended tempering treatment for two weeks. This observation might give new insights into microstructure formation and deformation of metallic alloys.

MM 52.4 Wed 17:45 IFW B

Diffusion Brazing of γ-TiAl Alloys: Comparison of Microstructure Development and Mechanical Strength for Two Different Brazing Solders — •Katja Hauschildt, Andreas Stark, Norbert Schell, Florian Pyczak, and Martin Müller — Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

TiAl alloys are increasingly used as light weight material, for example in aero engines, which also leads to a request for suitable repair methods. For this purpose, diffusion brazing is a promising method for the closure of cracks (in noncritical or not highly loaded areas) as it is already used for Ni-base superalloys. Therefore, two different brazing solders based on Ti-Fe and Ti-Ni were investigated for joining the alloy Ti-45Al-5Nb-0.2B-0.2C (in at. %). Tensile tests at room temperature show different mechanical strength depending on the brazing solder. Furthermore, the phases and their development and distribution over the brazing zone were investigated time and space resolved during the brazing process. Here, the two brazing solders show differences in development and fraction of the phases. These analyses were performed with high-energy X-ray diffraction using the HZG-run materials science beamline HEMS at the synchrotron radiation facility at DESY in Hamburg, Germany. In addition, analysis with electron microscopy and electron backscatter diffraction show significantly different grain sizes in the brazed region for both brazing solders. The results of phase analysis and electron backscatter diffraction can be combined to explain the different microstructure after the brazing process and thus the different mechanical strength depending on the two brazing solders.

MM 53: Invited talk Maier-Kiener

Time: Wednesday 18:30–19:00 Location: BAR 205

Invited Talk MM 53.1 Wed 18:30 BAR 205
Small scale deformation behavior of high performance materials - Advanced mechanical testing meets high end microstructure characterization — •Verena Maier-Kiener, Irmgard Weissensteiner, Benjamin Schuh, Anton Hohenwarter, and Helmut Clemens — Montanuniversität Leoben, Austria

Alloy design for modern high performance materials requires exact knowledge of the microstructure evolution during processing, but also a fundamental in-depth knowledge of the dominating deformation mechanism. Therefore, a direct combination of advanced microstructural characterization techniques with sophisticated micromechanical testing under various conditions is required. In the first part the potential of nanoindentation as a high throughput screening technique for probing phase decompositions in novel HEAs will be demonstrated. Together with APT studies it is shown that an increase in the Young's Modulus after various heat treatments in highly deformed conditions can be correlated to a phase decomposition of the initially single phase HEA into a multi-phase composite. The second part will focus on a CoCrW alloy used for biomedical application. Under mechanical loading, these alloys tend to a strain-induced martensitic transformation. In our studies, we combined macroscopic mechanical tests using a deformation dilatometer with small scale in-situ high temperature nanoindentation and high resolution EBSD analysis. This approach allowed the quantification of the onset strain for phase transformations, and further scale bridging insights regarding the influence of deformation rate and temperature on the plastic flow behavior.

MM 54: Invited talk Urban

Time: Thursday 9:30–10:00 Location: BAR 205

Invited Talk MM 54.1 Thu 9:30 BAR 205
Revealing the mechanism of Z-phase formation in 12% Cr ferritic-martensitic steels — •Daniel F. Urban and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

The objective of increasing the efficiency of fossil-fired power plants by raising the steam inlet temperature calls for ferritic-martensitic creep-resistant steels with a Cr content higher than 9% in order to achieve sufficient corrosion and oxidation resistance. However, it has been found that for 11-12% Cr steels strengthened by fine (V,Nb)N particles, these precipitates transform during long-term service into coarse, thermodynamically more stable Z-phase particles, CrMN (M=V,Nb,Ta), that deteriorate the steels mechanical behavior. We present extensive atomistic simulations, using density functional theory, that shed light on the essential mechanisms underlying the formation of the detrimental Z-phases and help to understand their respective dependencies. Our results reveal that the Z-phase transformation proceeds via diffusion of Cr atoms into the MN particles and their subsequent clustering in a layered arrangement of the Z-phase. We systematically scan the configuration space of various intermediate structures by varying their morphology, stoichiometry and point defect concentration. Our results support the ongoing experimental efforts to control the precipitation of the Z-phase through appropriate microstructural engineering and to exploit a fine distribution of the Z-phase itself as strengthening agent in the newly developed 12% Cr steel.

MM 55: Topical session: Data driven materials design - structure maps

Time: Thursday 10:15–11:45 Location: BAR 205

MM 55.1 Thu 10:15 BAR 205
Materials discovery with artificial intelligence — •Gareth Conduit and Philipp Verpoort — Department of Physics, University of Cambridge, UK

We have developed a computational tool that employs deep learning with neural networks to discover new materials. The tool combines databases of experimental results with Density Functional Theory calculations to get high accuracy across a broad range of compositions. This enables us to propose materials that are most likely to fulfil multivariate targets. This holistic approach to materials design has allowed us to propose four new nickel-base alloys for use in jet engines, whose properties have been experimentally verified, new Lithium-ion battery cathode materials, and titanium alloys.

The neural network approach to materials modelling can also assess the integrity of materials data. We have exploited this capability to automatically validate and correct entries in a commercial metal alloy and polymer database.

MM 55.2 Thu 10:30 BAR 205
Quantification of different atomic environments by a 2d structure map — •Jan Jenke[1], Aparna Puchakayala Appaiah Subramanyam[1], Thomas Hammerschmidt[1], David G. Pettifor[2], and Ralf Drautz[1] — [1]ICAMS Ruhr-Universität Bochum, Bochum, Germany — [2]University of Oxford, Oxford, United Kingdom

The assessment of the geometric (dis)similarity of crystal structures is a central requirement to facilitate information on structural stability with applications ranging from machine-learning of DFT data to the development of effective interaction models. The moments theorem relates the moments of the local electronic density of states to the local geometric environment of an atom. The moments of the electronic density of states therefore may be viewed as descriptors from which the local atomic surrounding of an atom may be reconstructed. By restricting our analysis to the two most important moments we map the phase space of possible atomic surroundings onto a two-dimensional space. Each local atomic environment corresponds to a point on the map and the entirety of all atomic environments forms a two-dimensional structure map. We apply the structure map to determine differences in the local atomic surrounding of known crystal structures, random structures, transformation paths and molecular dynamics trajectories. We show that our two-dimensional structure map leads to a natural separation of crystal structures that one would argue are very different while crystal structures that are similar are grouped close together. We suggest that our structure map is able to sample the space of atomic surroundings in a formal locally but at the same time intuitive way.

MM 55.3 Thu 10:45 BAR 205
Uncovering structure-property relationships of materials by subgroup discovery — •Mario Boley[2], Bryan R. Goldsmith[1], Jilles Vreeken[2], Matthias Scheffler[1], and Luca M Ghiringhelli[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Max Planck Institute for Informatics, Campus Mitte, 66123 Saarbrücken, Germany

Data analytics applied to materials-science data often focuses on the inference of a global prediction model for some physical or chemical property of interest for a given class of materials, such as activation barriers or binding energies. However, the underlying mechanism for some target property could differ for different materials within a large pool of materials-science data. Consequently, a global model fitted to the entire dataset may be difficult to interpret and may well hide or incorrectly describe the actuating physical mechanisms. In these situations, local models would be advantageous to global models. Subgroup discovery (SGD) is presented here as a data-mining approach to find interpretable local models of a target property in materials-science data. We first demonstrate that SGD can identify physically meaningful models that classify the crystal structures of 82 octet binary semiconductors as either rocksalt or zincblende. The SGD framework is subsequently applied to 24 400 configurations of neutral gas-phase gold clusters with 5 to 14 atoms to discern general patterns between geometrical and physicochemical properties. This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Center of Excellence.

MM 55.4 Thu 11:00 BAR 205

Predicting lattice parameters of ternary compounds by compressed sensing — •Benedikt Hoock^{1,2}, Santiago Rigamonti^{1}, Luca Ghiringhelli^{2}, Matthias Scheffler^{1,2}, and Claudia Draxl^{1,2} — ^{1}Humboldt-Universität zu Berlin — ^{2}Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Data analytics is emerging as a new branch of materials science enabling the interpolation and even (moderate) extrapolation of high-level computational results. In our present work, we demonstrate the successful prediction of lattice parameters for a set of 438 group-IV zincblende ternary compounds from density-functional theory (DFT) results. We use a compressed-sensing based method that combines the least absolute shrinkage and selection operator (LASSO) and ℓ_0-regularized optimization on a feature space consisting of basic features and a large range of simple mathematical combinations of them. The basic features comprise atomic and dimer DFT data as well as properties of relaxed tetrahedral clusters. We achieve a root mean square error of ~ 0.04 Å(~ 0.4 %) for the fit and a similar prediction accuracy, as estimated by a leave-10%-out cross-validation.

MM 55.5 Thu 11:15 BAR 205

Compressed-Sensing Models for the Prediction of the (Meta-)Stability of Octet Binaries — •Emre Ahmetcik, Runhai Ouyang, Christian Carbogno, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

Predicting the ground-state and metastable crystal structures of materials from just knowing their composition is perhaps the most important challenge in materials science. In a recent showcase study [1], a compressed-sensing based methodology was introduced to identify the *descriptors* (nonlinear functions of atomic input features) that best describe and predict the relative stability of zincblende versus rocksalt octet binary compounds. In this work, we have extended this approach to describe the relative stability and energy differences between eight different polymorphs of the octet binary materials, so that an accurate prediction of their ground and metastable states becomes possible. We discuss how this is tackled by introducing a new class of descriptors that map the geometry of different structures into a well defined scalar (the “reduced” Madelung energy) and a multi-objective optimization (the simultaneous minimization of the prediction error of all formation-energy differences among the eight considered polymorphs).

This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

[1] Ghiringhelli *et al.*, PRL **114**, 105503 (2015).

MM 55.6 Thu 11:30 BAR 205

Self-organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun, Michael Fernandez, and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-art of Deep Learning (DL) algorithm are having tremendous impact on Big Data analytics across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between data of nanomaterial*s quantum chemistry information and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a data structure that could be suitable for artificial neural networks. At the Molecular & Materials Modelling Laboratory we are evaluating the efficiency of visualising nanoparticles’ 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and their modelling with DL framework. Self-organisation Map (SOM) classifies high-dimensional data into low-dimensional space without supervision, while retaining the intrinsic topological relationship of the dataset. This algorithm is ideal for representing 3D molecular electrostatic potential surface (EPS) with a single 2D snapshot. The 2D image could possibly be fed into conventional classifier models, to correlation the EPS with other corresponding chemical properties of the molecules.

MM 56: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses - kinetic transitions

Time: Thursday 10:15–11:30 Location: IFW A

Topical Talk MM 56.1 Thu 10:15 IFW A

anomalous atomic motion in metallic glasses revealed by coherent X-rays — •Beatrice Ruta — Institute of Light and Matter, Lyon 1 University-CNRS, France.

Metallic glasses display outstanding thermal, mechanical and chemical properties, which make them forefront materials for technological applications in many diverse fields such as medicine, environmental science and engineering. Their widespread use is, however, limited by their lack of stability over time due to ongoing relaxation processes and physical aging. X-ray Photon Correlation Spectroscopy (XPCS) has recently emerged as the very only technique able to measure the atomic motion in both crystalline and amorphous materials. By collecting series of diffraction data with coherent X-rays, XPCS measures the particle dynamics though the temporal evolution of the intensity fluctuations in the generated speckles patterns. Measurements on metallic glasses have revealed the existence of microscopic structural rearrangements, which cannot be explained by any current theory. In these systems, the dynamics evolves from a diffusive atomic motion in the supercooled liquid phase to a stress-dominated dynamics in the glass, characterized by a complex hierarchy of aging regimes. By combining dynamical (XPCS) and structural (XRD) studies we have been able to quantitatively link for the first time this anomalous atomic motion to microscopic structural mechanisms usually observed in diffraction studies, providing a broader unique view of the glassy state.

MM 56.2 Thu 10:45 IFW A

Structural origins of the boson peak in metals: From high-entropy alloys to metallic glasses — •Karsten Albe, Tobias Brink, and Leonie Koch — Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Germany

Virtually all amorphous materials exhibit a boson peak, which is an excess of vibrational modes at low frequencies compared to the phonon spectrum of the corresponding crystal. Until recently, the consensus was that it originated from “defects” in the glass. However, the boson peak was also attributed to the first van Hove singularity of crystal lattices in alternative theories. A recent viewpoint is that the van Hove singularity is simply shifted by the decreased density of the amorphous state and is therefore not a glass-specific anomaly. In the current contribution, we aim to resolve this question for metallic systems. Using molecular dynamics computer simulations of high-entropy alloys and metallic glasses of the same composition, we show that the boson peak consists of additional modes which only arise in structurally disordered, softened regions [1]. Consistent with theoretical models, these regions are characterized by reduced stiffness and can be regarded as “soft spots”: The boson peak can serve as an indicator for the amount of such regions. This is consistent with observations that find an increased boson peak signal in mechanically deformed glasses in which an increase of the boson peak originates in the shear band [2].

[1] Brink *et al.*, PRB, accepted (2016)
[2] Bünz *et al.*, PRL **112**, 135501 (2014)

MM 56.3 Thu 11:00 IFW A

Fragile-strong liquid transitions and the underlying structural transitions in chalcogenide glassformer Ge15Te85 and bulk metallic glass-forming liquids — •Shuai Wei^{1}, Moritz Stolpe^{2}, Oliver Gross^{2}, William Hembree^{2}, Simon Hechler^{2}, Jozef Bednarcik^{3}, Ralf Busch^{2}, Pierre Lucas^{4}, and C.Austen

Angell[4] — [1]Arizona State University, Tempe, USA — [2]Saarland University, Saarbruecken, Germany — [3]DESY, Hamburg, Germany — [4]University of Arizona, Tucson, USA

A striking anomaly in the viscosity of chalcogenide glass-forming alloy Ge15Te85 is reminiscent of the equally striking comparison of liquid tellurium and water. Applying the Adam-Gibbs viscosity equation to calorimetric data, we find a fragile-to-strong liquid transition (FS-transition), and then predict the "strong" liquid course of the viscosity down to Tg at 406 K. The extrapolation is in good agreement with a direct measurement of fragility near Tg using differential scanning calorimetry. The in-situ X-ray scattering data reveal that the transition is not only related to short-range-order (SRO) structural change, but also linked to a remarkable development of medium-range-order (MRO). The latter manifests as an emerging pre-peak in total structural factor S(Q) and an atomic pair correlation on the length scale of ~8 Å in the real-space G(r) function. The FS-transitions at high pressures are examined in terms of experimental data and the Ehrenfest relation. Finally, we compare the behavior of Ge15Te85 with the liquid-liquid transition in the bulk metallic glass-forming liquid, Zr58.5Cu15.6Ni12.8Al10.3Nb2.8 (Vit.106a).

MM 56.4 Thu 11:15 IFW A

Indications for a kinetic crossover in bulk metallic glasses — •Stefan Küchemann[1], Robert Maass[1], and Konrad Samwer[2] — [1]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, USA — [2]1. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

In the supercooled liquid, kinetic crossovers strongly alter the dynamics of glass-forming alloys leading, for instance, to the breakdown of the Stokes-Einstein relation and the emergence of a secondary relaxation mode. Measurements of the static structure factor during ultrafast heating experiments of metallic glasses reveal an underlying structural transition which occurs in the close vicinity of the kinetic crossover in the supercooled liquid [1]. In this contribution we provide evidence that a kinetic crossover also occurs in the glass state. By covering an extended range of heating rates from very slow to ultrafast we are able to show that the glass transition temperature as a function of heating rate deviates from the expected Vogel-Fulcher-Tamann behavior [2]. At this crossover the amorphous structure rejuvenates despite the exposure to elevated temperatures which changes the mechanical properties. The results are discussed in the framework of an underlying thermodynamic phase transition.

The authors acknowledge the financial support by the DFG within FOR1394 in P1.

[1] S. Küchemann and K. Samwer, Acta Materialia 104, 119 (2016).
[2] S. Küchemann, G. Gibbins, J. Corkerton, E. Brug, J. Ruebsam, and K. Samwer, Philosophical Magazine Letters, 1 (2016).

MM 57: Microstructure and Phase Transformations - transformation kinetics

Time: Thursday 10:15–11:15 Location: IFW B

MM 57.1 Thu 10:15 IFW B

Capturing the evolution of fractal abnormal grains in nanocrystalline $Pd_{90}Au_{10}$ — •Raphael Zeller[1], Harms Fey[1], Christian Braun[2], Philipp Romberger[1], Rainer Birringer[2], and Carl Krill[1] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

During abnormal grain growth, a bimodal size distribution is established by the rapid growth of a few grains to much larger sizes than their neighbors. Usually, such abnormal grains expand in all directions at roughly the same speed, but in nanocrystalline $Pd_{90}Au_{10}$, they appear to send out "tentacles" into the surrounding matrix, which ultimately results in highly irregular, fractal-like grain shapes. Exploiting the fast heating and cooling capabilities of a salt-bath furnace, we have investigated the evolution of fractal grain morphologies in nano-$Pd_{90}Au_{10}$, finding two surprises: higher temperatures sometimes lead to smaller grains, and longer annealing times do not necessarily promote further grain growth (but they can affect the fractal dimension of the grain shape). We discuss these results in the framework of standard growth models supplemented by ideas from nucleation theory.

MM 57.2 Thu 10:30 IFW B

Extracting the kinetics of grain growth in Al-based polycrystals from 4D measurements — •Mingyan Wang[1], Jules Dake[1], Jette Oddershede[2], Henning Sørensen[3], Søren Schmidt[2], and Carl Krill[1] — [1]Ulm University, Germany — [2]Technical University of Denmark, Denmark — [3]University of Copenhagen, Denmark

Conventional studies of grain growth rely on 2D micrographs, which reveal that curved grain boundaries (GBs) tend to migrate toward their centers of curvature. From bicrystal experiments we learn that the reduced mobility (the product of GB mobility and energy) depends not only on curvature but also on boundary misorientation and inclination. Using 3D x-ray diffraction (3DXRD) microscopy, we have investigated the latter dependency in Al-based polycrystalline materials following a novel 4D protocol. From a series of 3D snapshots separated by isothermal annealing intervals, we have extracted the morphology, misorientation and migration rate of more than ten thousand GBs in a single sample, forming the basis for a robust statistical analysis of local growth kinetics. In one particular specimen, the observed dependency of reduced mobility on misorientation and inclination is consistent with behavior expected of normal grain growth, but in another case we find evidence for abnormal boundary migration that does not fit standard models.

MM 57.3 Thu 10:45 IFW B

Steady state structure of the moving faceted grain boundaries — •Sherri Hadian, Blazej Grabowski, and Jörg Neugebauer — Department for Computational Materials Design, Max-Planck-Institut fu*r Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Du*sseldorf, Germany

Migration of grain boundaries in metals plays an important role in the evolution of the microstructure. To gain insight on dynamics of grain boundaries in realistic materials, we have studied the motion of grain boundaries of general orientations. These boundaries have been observed to facet on different length scales. We have studied the finite facet length effects on the mobility of grain boundaries using MD simulations and analytical models. Grain boundaries were run under different driving forces at a wide range of forces/temperatures and their kinetics and mechanisms of motion were thoroughly investigated. The results imply that for high driving forces the steady state structure of the moving boundaries differs from their static equilibrium structure.

MM 57.4 Thu 11:00 IFW B

Analysis of the melting and solidification behavior of Pb nanoparticles embedded in Al matrix with Ga addition — •Martin Peterlechner, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Germany

Melting and crystallization solidification of nanoparticles are of academic interest due to size effects. Nanoparticles embedded in a matrix show contributions to their melting behavior caused by the coherency of the interfaces and pressure of the matrix. In the present study, nanoparticles of the low melting point material Pb was were processed as nanoparticles embedded in an coarse grained Al matrix where with Ga contents up to 9 at% was addedin order to vary the misfit and thus the coherency of the interfaces. The embedded nanoparticles show a decreasing melting and solidification temperatures with increasing Ga contents, due to an atomistically flat decoupling wetting layer at the Al-Pb interface. In the present work, the Transmission electron microscopy (TEM) analysis is supported by multislice image simulations, showing a signal broadening of the TEM analysis at the interface. A reduced melting enthalpy is in agreement with a the observed layering effect. The results are discussed with respect to current models. reducing the effective volume of the melting species.

MM 58: Nanomaterials I

Time: Thursday 10:15–11:45 Location: IFW D

MM 58.1 Thu 10:15 IFW D

Factors Influencing Melting and Solidification of In-Nanoparticles Embedded in an Al-matrix — •Mostafa Mohamed, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics,Münster,Germany

Nano-crystalline Indium particles embedded in an Al-matrix are synthesized by rapid solidification. Calorimetry and electron microscopy was utilized to study the melting and solidification of In-nanoparticles with a diameter between 20-350 nm. The volume strains accompanying the transformation are accommodated partially by generation of dislocations and missing wedges of the nanoparticles. Thermal cycling leads to a reduction of the maximum overheating temperature, and an increase of the minimal solidification temperature. The three effects which can affect the equilibrium melting temperature of In-nanoparticles, change in volume during melting, differential thermal expansion of the nanoparticles and the matrix capillarity effect are discussed.

MM 58.2 Thu 10:30 IFW D

Nanoparticles and Nanocomposite Thin Films Prepared by Gas Aggregation Source — •Oleksandr Polonskyi, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Christian-Albrechts University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Nanocomposite thin films consisting of metal nanoparticles (NPs) in a dielectric organic or ceramic matrix have unique functional properties with numbers of applications. The metallic nanoparticles typically form via a self-organization during co-deposition of the metallic and matrix components. Various methods such as sputtering, evaporation, and plasma polymerization have been applied for the deposition of the matrix component, while the metallic component has mostly been sputter deposited. However, recently gas aggregation nanoparticle sources have attracted high interest in order to obtain independent control of filling factor and size distribution of the embedded metallic nanoparticles. In the present talk, the details about formation of nanoparticles and nanocomposites by means of gas aggregation method will be discussed. In addition, we report on the <<in-flight>> treatment of metallic nanoparticles, generated by gas aggregation method for novel nanostructure formation. Here, in particular, the attention will be paid to optical composites and silver containing biocompatible antibacterial coatings with tailored release rate.

MM 58.3 Thu 10:45 IFW D

Formation of Co/SiO2 nanocomposites via dewetting of multilayer structures — •Oleksandr Polonskyi, Justin Jetter, Carsten Hänel, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Christian-Albrechts University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Nanocomposite thin films with metallic nanoparticles embedded into dielectric matrix have attracted much attention for their interesting functional properties. In the current work, we focus on magnetic Co/SiO2 nanocomposites prepared via magnetron sputtering of Co-SiO2 multilayers and subsequent heat treatment, leading to formation of Co nanoparticles embedded in an SiO2 matrix via dewetting and self-organization. The influence of deposition parameters and heat treatment conditions on microstructure and properties of the resulting films was investigated. Structure and morphology of the samples were characterized by SEM and TEM. XPS was used to investigate the chemical composition of the deposited samples and for monitoring of the changes occurring during heat-treatment. Vibrating sample magnetometry (VMS) was applied for investigation of magnetic properties. The mechanism of the self-organized microstructural evolution will be discussed.

MM 58.4 Thu 11:00 IFW D

Quantitative heat capacity measurements of Au nanoparticles using a nanocalorimeter — •Emanuel Franke[1], David A. LaVan[2], and Cynthia A. Volkert[1] — [1]Inst. für Materialphysik, Uni Göttingen, 37077 — [2]MML, NIST, Gaithersburg, USA 20899

As sample length scales reach down to nanometers, and the surface influence becomes large, thermal properties such as the heat capacity change. The involved heat in such samples is very small and can only be measured via convent. calorimetry by pressing milligrams of sample material together, whereby the surface influence of the sample is reduced. However, nanoscale samples can be directly measured by MEMS-based differential nanocalorimeters which have sufficient res. to measure with nJ sensitivity. Nonetheless, it is well known that heat losses of the MEMS sensors may change in the presence of a sample, leading to large changes in the nanocalorimetric signal and quantitative determination of heat capacity. In this study, FEA is used to investigate the interplay of heat losses (rad. and cond.), sample properties (therm. emissivity and conductivity), and temp. distr. on the sensor. On the basis of this analysis, the influence of exp. issues (misaligned sample, amb. temp.) can be evaluated. Furthermore, the sample geometry could be adapted to minimize the influence of the sample prop. on the measurement. With this knowledge, the heat capacity of Au nanoparticles (1 nm to 20 nm) was measured from 30 K to 300 K with a heating rate of 18,000 K/s with a resolution of better than 1 nJ/K. Together with TEM investigations, this reveals an enhancement in the heat capacity at low temp. that decr. with incr. particle size.

MM 58.5 Thu 11:15 IFW D

Stability of carbon nanotubes under hydrostatic pressure investigated by Monte Carlo simulations — •Markus Hartmann — Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

Carbon nanostructures are a fascinating class of materials combining high stiffness with low weight and exceptional toughness that makes carbon a promising candidate for applications in structural mechanics. Understanding the mechanical properties of these structures on every length scale is of utmost importance to be able to exploit the full potential of these materials. Monte Carlo simulations are a perfect tool to gain an insight into the complex deformation behavior of carbon nanostructures like graphene [1], nanotubes [2] and fullerenes [3] on an atomic scale. In the presented work I will discuss investigations on the mechanical stability of carbon nanotubes under hydrostatic pressure. Carbon nanotubes of different sizes and chiralities will be investigated. The shape of the initially circular cross-section of the tubes will be monitored. Under increasing load it first ovalizes into an elliptic shape, upon further increase of the load the shape further evolves into a peanut-like shape. Finally I will discuss the effect of nanotube size on the critical collapse pressure.

[1] Hartmann et al., Europhys. Lett. 103, 68004 (2013)
[2] Sun et al., Proc. Appl. Math. Mech. 13, 7 (2013)
[3] Holec et al., Phys. Rev. B 81, 235403 (2010)

MM 58.6 Thu 11:30 IFW D

Alternative substrate materials for silicene: WSe_2 and MgX_2 (X = Cl, Br, and I) — •Udo Schwingenschlögl and Jiajie Zhu — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Silicene is the Si analogue of graphene with honeycomb structure and characteristic Dirac states, while being fully compatible with current Si-based nano-electronics. It can be prepared on metallic substrates, such as Ag(111), Ir(111) and ZrB_2(0001), but a strong interaction regrettably perturbes the electronic states. Semiconducting Si(111) and SiC(0001) substrates, on the other hand, require surface passivation due to dangling bonds, which complicates the preparation procedure. We employ first-principles calculations in order to identify alternative substrate materials, focussing on layered compounds, because a weak interaction with silicene is expected. Both WSe_2 and MgX_2 (X = Cl, Br and I) turn out to be interesting candidates. The effects of these substrates on the properties of silicene are analyzed and discussed with respect to technological requirements.

References:
- Journal of Materials Chemistry C **3**, 3946-3953 (2015)
- ACS Applied Materials & Interfaces **6**, 11675-11681 (2014)

MM 59: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI

Time: Thursday 10:30–13:45 Location: GER 38

MM 59.1 Thu 10:30 GER 38

Implicit solvation functionality in FHI-aims: Kirkwood multipole expansion model — •Markus Sinstein, Karsten Reuter, and Harald Oberhofer — Technische Universität München, Germany

Implicit solvation models describe a liquid environment in form of a dielectric continuum. Used within first-principles calculations for the solute such models provide a numerically most efficient way to effectively capture solvation effects. To this end we have implemented the multipole expansion (MPE) model introduced originally by Kirkwood into the full-potential density-functional theory (DFT) code FHI-aims. This implementation fully exploits the optimized multi-center multipole decomposition of the density performed within FHI-aims and therewith leads generally to an insignificant overhead as compared to the underlying DFT calculation for the solute.

Aiming to minimize the number of free parameters inevitably connected with such implicit models, we use an iso-density definition of the solvent cavity. As to the other parameters, we present an efficient parametrization scheme based on experimentally measured hydration energies of small organic molecules. Finally, we discuss extensions of the solvation model to address extended solid-liquid interfaces.

MM 59.2 Thu 10:45 GER 38

Using Dipsersion-Corrected Density Functional Theory to Understand the Phase Diagram of Alkanethiolates on Gold — •Joakim Löfgren, Henrik Grönbeck, Kasper Moth-Poulsen, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

A key challenge in modern computational materials chemistry is the description of van der Waals interactions in density functional theory simulations, where the failure of conventional exchange-correlation functionals is well-known. While, in the recent years, several methods have been proposed for overcoming these difficulties, the applications are becoming increasingly more demanding as well. An important example is that of ligand-protected nanoparticles, which typically feature metallic, covalent as well as dispersive interactions that should all, ideally, be treated on an equal footing. In this work we show that significant progress can be made in this direction: with the aid of the recently-developed vdW-DF-cx functional we study the phase diagram of self-assembled monolayers of alkanethiolates on gold. This system is important for practical applications and as a general representative of self-assembly at a metal surface. In particular, a quantitative description of the dispersion-driven phase transition between a lying-down and a standing-up monolayer is obtained using an ab inito thermodynamics framework. The results are shown to be in good agreement with experimental data and highlight that accurately accounting for dispersive interactions is both feasible and a crucial part of modeling self-assembled systems.

MM 59.3 Thu 11:00 GER 38

Finite-temperature properties of the thermoelectric clathrate $Ba_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Intermetallic clathrate compounds are promising candidates for high-efficiency thermoelectric (TE) applications. Here, we study $Ba_8Al_xSi_{46-x}$ in the composition range $x \in [6, 16]$ [1]. Recent theoretical studies [2] show a strong dependence of the electronic properties on configuration, i.e. the atomic arrangement of the substitutional Al atoms in the crystal framework. At the Zintl composition ($x = 16$), the ground-state configuration is semiconducting. However, configurations higher in energy are metallic. Understanding this metal-semiconductor transition is essential, as semiconducting behavior is a prerequisite for TE applications. In this work, we employ the cluster expansion technique combined with Monte-Carlo simulations and the Wang-Landau method [3] to access finite-temperature properties. We find that the transition is driven by a partial order-disorder transition of the substituents. Most importantly, it is found that the transition temperature ($\sim 800\,K$) at the Zintl composition is close to the typical temperatures at which the figure of merit of TE clathrates is maximal. Signatures of the transition in the entropy, order parameter, specific heat, and canonical distribution are analyzed for the full composition range.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)
[2] M. Troppenz, S. Rigamonti and C. Draxl; preprint.
[3] F. Wang and D. P. Landau, *Phys. Rev. Lett.* **86**, 2050 (2001)

MM 59.4 Thu 11:15 GER 38

Electronic structure and solid-state optical properties of indigo from time-dependent optimally tuned range-separated hybrid functional theory — •Bernd Kollmann[1], Arun Kumar Manna[2], Daniel Lüftner[1], Leeor Kronik[2], and Peter Puschnig[1] — [1]Institute of Physics, NAWI Graz, University of Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Indigo is a natural dye with a long history in organic chemistry. Recent applications of indigo as a functional building block for organic electronics, like in solar cells or field effect transistors, have renewed the interest in the chemical and physical properties of this molecule. We report on its electronic structure for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal phases. Further we investigate the optical properties of the bulk molecular crystal phases. For the molecule we employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory. Comparing the theoretical results obtained with different levels of theory and with experiment emphasizes the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. For the bulk crystals we take into account the screening in the bulk by using an optimally tuned screened range-separated hybrid (OT-SRSH) approach. Regarding the optical properties of the bulk molecular phases we employ time-dependent density functional theory (TDDFT) to calculate the absorption spectra, whereby TDDFT represents an accurate low-cost substitute to many-body perturbation theory.

MM 59.5 Thu 11:30 GER 38

Thermodynamic properties from ab-initio calculations - Ti as a case study — •Guy Makov — Materials Dept, Ben-Gurion University of the Negev, Beer Sheva, Israel

Ab-initio calculations of thermophysical properties and of phase stability as a function of pressure and temperature are considered in titanium as a case study. Ti is of interest due to its multiple phases and unusual thermophysical properties. At low temperatures Ti has been reported to exhibit negative anisotropic thermal expansion. In addition, there have been reports of two additional phases at high pressure and room temperature, and a possible transition to a bcc phase at very high pressures.

Despite extensive studies there remains both experimental and theoretical uncertainty in determining the phase diagrams and selected properties. Density Functional Theory total energy calculations complemented by Density Functional Perturbation Theory (DFPT) calculations of phonon spectra are obtained as a function of pressure. The free energy and thermal properties (heat capacity and thermal expansion) of Ti phases, phase equilibria and high pressure phase sequence are determined. The contribution of phonon modes to the thermal expansion is analyzed and the negative thermal expansion is shown to be dominated by negative mode Gruneisen parameters at specific points on the Brillouin zone boundaries. The elastic (Debye) theory for negative thermal expansion is shown to be irrelevant for these phenomena. Uncertainties in the calculated results are discussed in light of experimental observations & motivating further experimental studies.

MM 59.6 Thu 11:45 GER 38

Molecular orbitals in the bismuth perovskites — •Kateryna Foyevtsova[1,2], Arash Khazraie[1,2], Ilya Elfimov[1,2], and George A. Sawatzky[1,2] — [1]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1 — [2]Stewart Blusson Quantum Matter Institute, Vancouver, BC, Canada V6T 1Z4

The bismuth perovskites $SrBiO_3$ and $BaBiO_3$ become superconducting upon hole doping, with the transition temperatures as high as 30 K. The origin of the superconductivity in these compounds has remained unidentified for more than three decades. The BCS mechanism alone is not sufficient to account for such a high T_c due to the small electron-phonon coupling that is being consistently found in numerous experimental and theoretical studies. Further effects must therefore be of key importance, such as, for example, formation of bipolarons.

In this talk, we will focus on the insulating state of the pristine $SrBiO_3$. Peculiarly, this state is associated with a structural distortion whereby the Bi-O bonds disproportionate, resulting in a three-dimensional array of alternating small and large BiO_6 octahedra. This "breathing" distortion melts away with doping and is believed to be competing with superconductivity. We will show using DFT calculations that the microscopic state in the pristine bismuthates corresponds to a lattice of frozen bipolarons. More specifically, the holes, intrinsically present in the material, condense pairwise into the A_{1g}-symmetric molecular orbitals formed from the O-p_σ atomic orbitals of the small BiO_6 octahedra. This is facilitated by the strong hybridization between the O-2p states and the Bi-6s states.

MM 59.7 Thu 12:00 GER 38

Ab initio calculations and strain-dependent scaling of excitons in carbon nanotubes — •Christian Wagner[1,3], Jörg Schuster[2], Michael Schreiber[3], and André Schleife[4] — [1]Center for Microtechnologies, TU Chemnitz, Germany — [2]Fraunhofer Institute ENAS, Chemnitz, Germany — [3]Institute of Physics, TU Chemnitz, Germany — [4]Department for Materials Science, UIUC, USA

Optical transitions in carbon nanotubes (CNTs) show a strong strain sensitivity, which makes them suitable for optical strain sensing at the nano-scale and for strain-tunable emitters. The origin of this effect is the band-gap change, depending on strain and chirality, which is well explored. However, there is no quantitative model for the strain dependence of optical transitions — as they are subject to strong excitonic effects due to the quasi one-dimensional structure of CNTs.

One approach towards such a model is the scaling relation of CNT excitons with respect to dielectric constant, reduced mass, and CNT radius given by Perebeinos *et al.* However, the description of screening in this model is insufficient, since for CNTs, a one-dimensional wave-vector dependent dielectric function $\epsilon(q)$ is needed instead of an effective-medium dielectric constant ϵ_0.

We achieve this by combining the scaling relation with the wave-vector dependent screening model by Deslippe *et al.* The strain-dependent scaling is fitted to electronic-structure calculations within many-body perturbation theory as a reference. This enables us to quantitatively predict the strain dependence of optical transitions for any CNT.

MM 59.8 Thu 12:15 GER 38

Dzyaloshinskii-Moriya-interaction energy, where it is located? Real and reciprocal spaces views. — •Leonid Sandratskii — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Recently Dzyaloshinskii-Moriya interaction (DMI) attracted new wave of intense attention stimulated by its role in the stabilization and fast dynamics of skyrmions. Numerous approaches have been suggested for the estimation of the the DMI parameters. Many efforts are devoted to reveal the electronic properties responsible for the strength of the DMI and, in this way, to help to engineer the materials with desired DMI characteristics. Although there is full consensus with respect to the most fundamental reasons of the DMI, the SOC and broken inversion symmetry, in details the physical pictures suggested by different authors differ strongly. In particular, this concerns the role of the avoiding crossings in the electronic structure, the spatial location of the DMI energy, the role of the orbital moments. This stimulated us to perform detailed study of the DMI in CoPt bilayer focusing on the open questions. We used both the approximate calculations for spin spirals with arbitrary wave vectors and more precise but also more time and resources consuming full relativistic calculations for supercells with the magnetic structures of opposite chirality. The results of the calculations are presented and analyzed.

MM 59.9 Thu 12:30 GER 38

***Ab-initio* study of the Raman spectra of strained graphene** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman spectroscopy is an important non-destructive method for characterizing graphene-based materials. The main features of Raman spectra of pristine graphene are the first-order G-band at $\approx 1580\,\mathrm{cm}^{-1}$ and the dispersive second-order 2D-band at $\approx 2700\,\mathrm{cm}^{-1}$. In this work, we perform a systematic analysis on the effect of strain on both bands. All calculations are done using the full-potential all-electron code `exciting` [1]. Phonon properties are computed within the frozen-phonon approximation, the frequency-dependent dielectric tensor within the random-phase approximation. Raman-scattering intensities are calculated from vibrational matrix elements and derivatives of the dielectric tensor with respect to the phonon normal coordinates [2]. Under biaxial strain both Raman bands are shifted, while uniaxial strain leads to a splitting of the G-band by lifting the degeneracy of the optical in-plane Γ-point phonons. Further, we explore the effect of different types of inhomogeneous strain on the optical phonon frequencies and Raman-scattering intensities.

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

[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).

MM 59.10 Thu 12:45 GER 38

DFT meets Landau Theory: The High Pressure Phase Transition of Lead Titanate — •Andreas Tröster — Vienna University of Technology, Institute of Material Chemistry, Getreidemarkt 9 A-1060 Wien, Austria

Landau theory (LT) coupled to infinitesimal strain is a cornerstone of the theory of structural phase transitions. At high pressures, however, this approach breaks down due to the appearance of large strains and the accompanying nonlinear elastic energy contributions. In density functional theory (DFT), on the other hand, stress and strain are easy to control, but entropic effects are difficult to incorporate since DFT is a genuine zero temperature method. Recently we have shown how to combine the strengths of these two antipodal approaches by constructing a high pressure extension of conventional LT with the help of DFT. Essential for the success of this approach is the ab initio calculation of pressure-dependent elastic constants. This theory yields a concise numerical description of the high pressure phase transition in strontium titanate, and also allows to resolve a number of severe and long-standing discrepancies between the experimental data and the theoretical description of the ferroelectric high pressure phase transition of the perovskite lead titanate, a material which is also of considerable technological interest.

MM 59.11 Thu 13:00 GER 38

Ground-State and Excitation Properties of Orthorhombic $\mathbf{MAPbI_3}$ — •Claudia Rödl and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Hybrid organic-inorganic halide perovskites are one of the most promising candidates for the next generation of photovoltaic devices with high power-conversion efficiencies. Despite the amazing progress in device fabrication, many of the fundamental properties of these materials are not yet understood. The flexibility in composition of hybrid perovskites permits to tune physical properties like band gap, dielectric constant, or optical absorption which renders them interesting also from a fundamental point of view and for applications beyond photovoltaics. The most intensively studied compound, methylammonium lead iodide ($MAPbI_3$), condenses in a low-temperature orthorhombic phase which undergoes a phase transition to a tetragonal structure at 162.2 K and transforms into a cubic high-temperature phase above 327.4 K. These phase transitions go along with a change in the optical properties. Here, we focus on the orthorhombic phase of $MAPbI_3$. We have studied the ground-state atomic structure, and in particular the orientation of the MA^+ ion within the inorganic cage, within density-functional theory. We investigate the one-particle excitation properties (band gap, photoemission spectrum) within the GW approximation of many-body perturbation theory. Moreover, we calculate optical and loss spectra using time-dependent density-functional theory and solving the Bethe-Salpeter equation.

MM 59.12 Thu 13:15 GER 38

Structure, nonstoichiometry, and geometrical frustration of $\boldsymbol{\alpha}$-tetragonal boron — •Jens Kunstmann[1], Naoki Uemura[2], Hagen Eckert[1], and Koun Shirai[2] — [1]TU Dresden, Germany — [2]Osaka University, Japan

It is currently believed that boron in the α-tetragonal structure is not an elemental crystal. Here we contradict this view and resolve the structural and thermodynamic characteristics of pure α-tetragonal boron via density functional theory calculations. The conditions for stable covalent bonding are almost fulfilled at a stoichiometric composition B_{52}. This phase is an elemental crystals with geometrical frustration. Furthermore, our thermodynamic considerations show that small, positive deviations from the stoichiometric composition occur at finite temperatures. [Uemura, Shirai, Eckert, Kunstmann, Phys. Rev. B 93, 104101 (2016)]

MM 59.13 Thu 13:30 GER 38

Magnetic response properties of thin films using Kubo's linear response formalism — •Andreas Held, Sebastian Wimmer, Sergiy Mankovsky, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München

We have applied the fully relativistic spin-polarized Korringa-Kohn-Rostoker method to investigate various magnetic response properties of two-dimensional systems such as free-standing mono- and multilayers, surfaces and thin films on surfaces. Our approach is based on an implementation of Kubo's linear response formalism within the tight-binding (or screened) KKR framework that allows introducing layer-resolved response coefficients τ_{ij}^{IJ}. Extending previous work [1] focusing on the symmetric part of the electrical conductivity tensor, we are able to describe the full response tensors connected to charge and spin transport, Gilbert damping, spin-orbit torque and the Edelstein effect. An implementation of the Coherent Potential Approximation for layered systems allows the treatment of disorder effects including the Vertex Corrections to the response coefficients [2]. This can be used to study chemical disorder in alloys but also to include the effect of finite temperatures. For the latter the so-called Alloy-Analogy Model [3] is employed to treat vibrations and spin fluctuations.

[1] W.H. Butler *et al.*, *Phys. Rev. B* **52**, 13399 (1995). [2] W.H. Butler, *Phys. Rev. B* **31**, 3260 (1985); K. Palotás *et al.*, *Phys. Rev. B* **67**, 174404 (2003). [3] H. Ebert *et al.*, *Phys. Rev. B* **91**, 165132 (2015).

MM 60: Topical session: Data driven materials design - machine learning

Time: Thursday 12:00–13:15 Location: BAR 205

MM 60.1 Thu 12:00 BAR 205

Finding descriptors for material properties from billions of candidates via compressed sensing: accurate prediction of crystal structures and band gaps from only chemical composition — •Runhai Ouyang, Emre Ahmetcik, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Identifying the key physical parameters (termed descriptor) determining the target material properties is a critical step toward material discovery and rational design. Thus far, systematic methods for the descriptor identification are not well established. In particular, it has been suggested that good descriptors should both yield an accurate prediction and be physically interpretable [L. M. Ghiringhelli,*et al.*, PRL **114**, 105503 (2015)]. In this talk, we present a systematic scheme for descriptor identification based on sure independent screening [J. Fan and J. Lv, J. R. Statist. Soc. B **70**, 849 (2008)] and compressed sensing [E. Candès and M. B. Wakin, IEEE Signal Proc. Mag. **25**, 21 (2008)]. The scheme starts with automatic building of the "feature spaces", i.e. all offered candidate descriptors, and the feature space may contain billions of options. The employed combination of sure independent screening and compressed sensing provides an efficient scheme for identifying the best low-dimensional descriptor. The approach is demonstrated for the important problems of crystal-structure and band-gap prediction. This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

MM 60.2 Thu 12:15 BAR 205

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for a wide range of systems. Due to their high flexibility, they allow to interpolate reference energies and forces obtained from electronic structure calculations, without the introduction of any constraint to the functional form. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy surface of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased by employing the EVB method to combine smaller fragments in a physically meaningful way. Preliminary results will be discussed and compared to density functional theory data.

MM 60.3 Thu 12:30 BAR 205

Automatic crystal-structure classification using X-ray diffraction patterns and convolutional neural networks — •Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

With the advent of high-throughput materials science, millions of calculations are now available to the scientific community (http://nomad-repository.eu and references therein). A reliable identification of the lattice symmetry in these calculations is a crucial first step for materials characterization and analytics. Current methods based on space-group symmetries require a user-specified threshold, and are unable to detect "average" symmetries for defective structures (e.g., with point defects, and/or strain). We propose a new machine-learning based approach to automatically classify periodic structures according to their Bravais lattice. First, we calculate the X-ray diffraction patterns, from which a classifying model is then learned using a convolutional neural network. This method is applied to crystal-structure classification of 3d, 4d, and 5d transition metal alloys, also containing vacancies. We show that our deep-learning model can correctly classify more than 99% of the crystal structures. Moreover, contrarily to other (common) methods, it does not require any tolerance threshold and provides a reliable probabilistic classification also for heavily defective structures. Our approach has been implemented in the NOMADsim package of the Novel Materials Discovery (NOMAD) Analytics-Toolkit (https://analytics-toolkit.nomad-coe.eu). This work received funding from the NOMAD Laboratory, a European Center of Excellence.

MM 60.4 Thu 12:45 BAR 205

Optimizing Materials Properties with Machine Learning Techniques: A Case Study on Hard-Magnetic Phases — •Johannes J. Möller, Georg Krugel, Wolfgang Körner, Daniel F. Urban, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Machine Learning (ML) is an emerging field in materials science, in which a numerical model is built in order to predict a certain feature, for instance a materials property. The model building is typically based on a (large) data set of e.g. crystal structures or chemical compositions, for which the property is already known. The beauty of this approach is that it not only allows us to predict the properties for unknown compositions, but also to determine the composition that optimizes the desired property. Furthermore, ML models are inherently independent of how the original input data sets were determined, i.e. by experiments or by simulations.

In this presentation, we use ML techniques to predict optimal chemical compositions for new hard-magnetic materials. The underlying data set was determined in a combinatorial high-throughput-screening approach based on density-functional theory calculations [Drebov et al., New J. Phys. 15 (2013); Körner et al., Sci. Rep. 6 (2016)]. The developed ML models allow us to predict promising structure-composition combinations for substitutes of state-of-the-art materials like $Nd_2Fe_{14}B$ with similar intrinsic ferromagnetic properties but no or less amounts of critical rare-earth elements. Finally, we discuss possible perspectives for further applications of ML in materials science.

MM 60.5 Thu 13:00 BAR 205

A theoretical tool to predict the nature of the 4f states of Ce compounds — •Heike C. Herper[1], Tofiq Ahmed[2], John M. Wills[2], Igor di Marco[1], Inka Locht[1], Anna Delin[3], Alexander V. Balasky[2], and Olle Eriksson[1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Center for Integrated Nanotechnologies, LANL, USA — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Cerium is the most abundant rare earth. Ce compounds are used in many applications and therefore different materials properties are needed. Since these properties are widely determined by the electronic structure the understanding of the degree of localization of the 4f electron is essential. Aiming to classify the Ce compounds regarding to their itinerant character we studied the hybridization function Δ of more than 350 data sets taken from the ICSD. The hybridization function has been calculated from first principles using a full-potential code [1]. We show that the strength of Δ evaluated in this way allows conclusions about the level of 4f localiztion. The results are consistent with the experimental information regarding the degree of 4f localization, for the studied materials. A strong anti-correlation between the size of Δ and the volume of the systems has been observed. The information entropy is about 0.42 which means a high predictive power that could be used to tailor new materials with desired properties.

[1] J. M. Wills et al, Full-Potential Electronic Structure Method, Springer series solid state science **167** (2010).

This work is supported by STandUP for energy (Sweden).

MM 61: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses V - dynamical response

Time: Thursday 11:45–13:15 Location: IFW A

Topical Talk MM 61.1 Thu 11:45 IFW A

Towards a dissipative atomic-scale theory of the dynamical response of metallic glasses — •Alessio Zaccone — University of Cambridge, U.K.

One of the most fruitful concepts to characterize the deformation of metallic glasses has been that of nonaffine displacements [1]-[3], defined as additional atomic motions on top of the affine displacements prescribed by the macroscopic strain tensor. Using this, and recognizing that nonaffine displacements ultimately originate from the breaking of local centrosymmetry on every atom in the amorphous lattice [4], opens up the possibility of formulating a "nonaffine lattice dynamics" of metallic glasses. I will show that new viscoelastic sum-rules can be derived from a system-bath Hamiltonian of the Zwanzig-Caldeira-Leggett type which leads to a low-temperature Generalized Langevin Equation for dissipative nonaffine motions. This approach can be combined with a mode-coupling result [5] for the atomic-scale damping coefficient (a non-Markovian friction which accounts for memory-effects) to give predictions of dynamic response in agreement with experimental results of mechanical spectroscopy. The approach also provides a robust connection with the vibrational density of states. Finally, a possible route to explain the beta-relaxation process with this approach is outlined.

[1] A. Zaccone & E. Scossa-Romano, Phys. Rev. B (2011). [2] T.C. Hufnagel, C.A. Schuh, M.L. Falk, Acta Mater. (2016). [3] S. V. Ketov, Y.H. Sun, et al., Nature (2015). [4] R. Milkus and A. Zaccone, Phys. Rev. B (2016). [5] L. Sjoegren and A. Sjoelander, J. Phys. C: Solid State Phys. (1979).

MM 61.2 Thu 12:15 IFW A

Plastic deformation mechanism of metallic glasses — •Vitalij Hieronymus-Schmidt[1], Harald Rösner[1], Alessio Zaccone[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Deutschland — [2]University of Cambridge, Cambridge, U.K.

Deformation of metallic glasses performed well below the glass transition temperature leads to the formation of shear bands, narrow regions in which the plastic flow is confined. It is believed that shear banding originates from individual stress concentrators having quadrupolar stress symmetry. To elucidate the underlying mechanisms of shear band formation, microstructural investigations were carried out on sheared zones using transmission electron microscopy. An evidence of a characteristic signature present in shear bands manifested in the form of sinusoidal density variations was found. On this basis we present an analytical solution for the observed post-deformation state derived from continuum mechanics using an alignment of quadrupolar stress field perturbations for the plastic events. Since we observe qualitatively similar features for three different types of metallic glasses that span the entire range of characteristic properties of metallic glasses, we suggest that the reported deformation behavior is generic for all metallic glasses, and thus has far-reaching consequences for the deformation behavior of amorphous solids in general.

MM 61.3 Thu 12:30 IFW A

The Effect of Glass Structure, Stress State and Strain Rate on Shear and Densification - A Nanomechanical Study on a Sodium-Boro-Silicate Glass — •Christoffer Zehnder[1], Niklas Peltzer[1], Doris Möncke[2], James Gibson[1], and Sandra Korte-Kerzel[1] — [1]RWTH Aachen University, Germany — [2]Alfred University, New York, USA

It is well known that the mechanical properties of glasses are closely related to their atomic structure. The exact structure-property-relationship, however, is only poorly understood even for fundamental mechanisms like shear and densification. Nanomechanical test methods like micropillar compression and nano-impact indentation can help fill this gap. In this study a sodium-boro-silicate glass is quenched from different temperatures to induce changes in the atomic structure. Micropillar compression was used to investigate the effect of uniaxial stresses and nanoindentation with different tip geometries enabled testing under different amounts of hydrostatic pressure. Finally, impact nanoindentation was utilised to observe the effect of high strain rates on the deformation of glass. It is shown that by changing the glass structure or the stress state one can influence the occurrence of shear and densification. Testing with different strain rates also revealed a strong strain rate dependence of the deformation mechanism. These findings are analysed against the background of the glass structure. The experimental techniques and analyses presented could easily be applied also to metallic glasses in order to investigate the effects of rate and stress state on their plastic deformation.

MM 61.4 Thu 12:45 IFW A

Yielding transition in a binary model glass under oscillatory shear: Molecular Dynamics computer simulation — •Juergen Horbach[1], Gaurav Prakash Shrivastav[1], and Pinaki Chaudhuri[2] — [1]Institut für Theoretische Physik II, Universität Düsseldorf, Germany — [2]The Institute of Mathematical Sciences, Chennai, India

Under shear, a glass may exhibit the transition from an elastically deformed state to plastic flow. The nature of the yield point at which this transition occurs is a highly debated issue. We use molecular dynamics simulation to study a model of a $Ni_{80}P_{20}$ glass under oscillatory shear. Recently, we have shown that the yielding in this system can be associated with a directed percolation transition of mobile regions [1-3]. Under oscillatory shear, the occurrence of a yielding transition depends on the maximal strain amplitude, γ_{max}, in each cycle. We show that the time scale at which the transition occurs diverges at a finite value of γ_{max}.

[1] G. P. Shrivastav, P. Chaudhuri, and J.Horbach, Phys. Rev. E **94**, 042605 (2016).

[2] G. P. Shrivastav, P. Chaudhuri, and J. Horbach, J. Rheol. **60**, 835 (2016).

[3] I. Binkowski, G. P. Shrivastav, J. Horbach, S. V. Divinski, and G. Wilde, Acta Mater. **109**, 330 (2016).

MM 61.5 Thu 13:00 IFW A

Effect of hydrogen on the pop-in behavior in a metallic glass — •Lin Tian, Moritz Hirsbrunner, Dominik Tönnies, and Cynthia Volkert — Institute of Materials Physics, University of Göttingen

Hydrogen is a detrimental element in structural materials which usually causes obvious reduction of fracture toughness. For example, hydrogen embrittlement is a well-known reason for failure of steels. In contrast, in metallic glasses, which are considered to be brittle materials, hydrogen (H) can play a beneficial roll by preventing shear band formation. In this contribution, the effect of H content on the pop-in behavior of a Zr based metallic glass (M) is studied. Samples are charged to different H content (H/M) with electrochemical hydrogen loading. Then, nanoindention with a spherical indenter is carried out on the surface of the samples. While the load of the first pop-in increases with increasing H content, the possibility of pop-ins occurring decreases. A transition from shear band dominated to homogeneous deformation is observed. This result is consistent with a study of the compression of submicron pillars in hydrogen gas environment. The suppression of shear band initiation is attributed to changes in the local environment induced by H doping, such as local strain.

MM 62: Microstructure and Phase Transformations - nucleation kinetics and pressure effects

Time: Thursday 11:45–13:00 Location: IFW B

MM 62.1 Thu 11:45 IFW B

Crystallization behavior of the Al86Ni8Y6 metallic glass forming alloy upon rapid cooling — •Alexander Kuball, Moritz Stolpe, and Ralf Busch — Saarland University, Chair of Metallic Materials, Saarbrücken, Germany

In this study, the crystallization behavior of Al86Ni8Y6 upon rapid cooling from the equilibrium melt is investigated and the crystalline phases that compete with the glass formation are identified. Al86Ni8Y6 is one of the best glass formers in the ternary Al-Ni-Y system. Contrary to previous studies suggesting α-Al as the primary phase upon quenching, this study reveals that glass formation is strongly restricted by the formation of the primary precipitating ternary intermetallic compound Al23Ni6Y4. The nucleation of Al23Ni6Y4 appears to be triggered by yttrium oxide particles present in the melt acting as heterogeneous nucleation sites. Once the primary phase Al23Ni6Y4 has been formed, further crystallization of the Ni and Y depleted melt occurs as α-Al. The corresponding results are shown and discussed with respect to their effects on the glass formation.

MM 62.2 Thu 12:00 IFW B

Can homogenous nucleation be controlled in a metallic glass? — •Bin Yang[1], Yulai Gao[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Albert-Einstein Str. 23-24, 18051 Rostock, Germany — [2]State Key Laboratory of Advanced Special Steels, Shanghai University, 149 Yanchang Road, 200072 Shanghai, PR China

Fast scanning chip calorimetry was successfully employed to not only suppress crystallization but also bypass homogeneous nucleation of an Au-based bulk metallic glass on controlled fast quenching. A truly amorphous metallic glass without homogeneous nucleation was acquired. Following the rapid quenching, annealing at different temperatures from 0.001 s to 10000 s was realized, in which homogeneous nucleation was allowed and various local-configurations were obtained consequently. Its effect on crystallization was quantified based on the evolution of enthalpy employing Tammann's two stage nuclei development approach. Finally, a C-curve illustrating the homogeneous nucleation kinetics was obtained and added to the conventional TTT diagram, by which a truly amorphous state and the kinetics of homogeneous nucleation can be estimated. The art to control homogeneous nucleation and the science to uncover the corresponding mechanism provide new insights how to tune the micro- to nano-structure of metallic glasses, and facilitates the understanding of solidification and glass forming ability both in engineering and scientific fields.

MM 62.3 Thu 12:15 IFW B

Thin interface asymptotics in the presence of convection for diffuse interface models of solidification — •Amol Subhedar, Fathollah Varnik, and Ingo Steinbach — ICAMS, Ruhr Universität Bochum, Germany

As a major transport mechanism, convection plays a critical role in the solidification phenomena. Here, the influence of convection on diffuse interface models of solidification is investigated both analytically and via numerical simulations. It is shown that results of the diffuse interface width become independent of the auxiliary interface width, as also shown in the absence of flow (A. Karma and W. Rappel, Phys. Rev. E, 53, p. 4323 (1996)). Analytic predictions are found to be quantitatively in line with the results obtained from extensive numerical simulations for various fluid-solid coupling schemes. This underlines the generic character of the results and highlights the broad range of its applicability to various available models of solidification in the presence of flow [A. Subhedar, I. Steinbach, F. Varnik, in preparation].

MM 62.4 Thu 12:30 IFW B

High Pressure Structural Phase Transition in NdX (X=P, As, Sb): A Density Functional Theory Study — •sanjay kumar singh[1,2], rishi singh[2], and ajay mittal[3] — [1]Department of Physics, Computational Material Physics Group, Aryabhatta Group of Institutes, NH-71, Bajakhana Road, Barnala - 148101, Punjab; India — [2]Department of Physics, S. S. V. Degree College, Hapur, C. C. S. University, Meerut, India — [3]Department of Mathematics, Aryabhatta Group of Institutes, NH-71, Bajakhana Road, Barnala - 148101, Punjab; India

The structural and phase transition properties of NdX (X = P, As, Sb) under high pressure have been investigated using an ab-initio full potential linear augmented plane wave plus local orbitals approach within the framework of density functional theory as implanted in the WIEN2k package. In this approach the generalized gradient approximation is chosen for the exchange-correlation functional energy optimization for calculating the total energy. At ambient conditions NdX stabilize in NaCl (B1 phase) structure. Under compression, it undergoes first-order structural transition from Fm-3m to P4/mmm (body centre tetragonal) phase at 30.0, 24.06 and 15.1 GPa which is found to be in good agreement with the available experimental data 30.0, 24.2 and 15.0 GPa respectively. The structural properties viz., equilibrium lattice constants, bulk modulus and its pressure derivative and volume collapse are also calculated and compared with previous calculations and available experimental data.

MM 62.5 Thu 12:45 IFW B

Pressure-induced ferroelastic phase transition in SnO_2 from density functional theory — •Lei Yang, Weiliu Fan, Yanlu Li, Lei Wei, and Xian Zhao — Shandong University

We studied the high-pressure ferroelastic transition of rutile- to $CaCl_2$-type SnO_2 within density functional theory and Landau free energy theory. Softening mechanism of B_{1g} mode (order parameter Q) and the coupling mechanism between the soft B_{1g} mode and the soft transverse acoustic (TA) mode (strain ε) are clarified by calculating Landau energy map around the ground state. It is found that the Sn-O-Sn bending induced soft B_{1g} mode effectively reduces the excess energy increase caused by bond stretching, which however always leads to SnO_6 octahedral distortion. The octahedral distortion is subsequently minimized by lattice distortion strain ε, which interacts with the soft B_{1g} mode to further increase the stability of system.

MM 63: Nanomaterials II

Time: Thursday 12:00–13:30 Location: IFW D

MM 63.1 Thu 12:00 IFW D

Nanoplasmonics from large-scale ab initio calculations: opposite trends in Ag and Na clusters — •Marc Barbry[1], Peter Koval[2], Natalia E. Koval[1], Javier Aizpurua[1], and Daniel Sánchez[1,2] — [1]Material Physics Center, San Sebastián, Spain — [2]Donostia International Physics Center, San Sebastián, Spain

An accurate description of electronic excitations is indispensable for understanding material properties and designing nanoscale devices. For instance, using large-scale TDDFT calculations, we have recently demonstrated the importance of taking into account the details of the atomic-scale structure [1] and the quantization of electron transport [2] in metal nanostructures in order to accurately describe their plasmonic properties. In this contribution we will compare the surface plasmon resonance of sodium and silver clusters within the same framework of *iterative* TDDFT [3]. Recent progress in our implementation made it possible to perform calculations of large clusters of diameters ranging from a few Å to 4–5 nm, counting up to 5000 silver atoms and using only modest computational resources (a 32-core node with 500GB RAM). With these new capabilities, we have characterized the size-scaling of the SPR frequency for both sodium and silver clusters. As expected these two materials show opposite behaviours that can be related to the different spill out of charge at the surface and to the additional screening created by the 4*d* electrons in silver.

[1] M. Barbry *et al.* *Nano Letters*, **15** (2015) 3410. [2] F. Marchesin *et al.* *ACS Photonics*, **3** (2016) 269. [3] P. Koval *et al.* *J. Phys.: Condens. Matter*, **28** (2016) 214001.

MM 63.2 Thu 12:15 IFW D

Ein-Photon-Ein-Elektron-Resonanz zur Interpretation der Spektren formanisotroper Nanopartikel aus mikrofluidischer Synthese — •Michael Köhler, Danja Kuhfuss und Andrea Knauer — TU Ilmenau, Inst. für Mikro- und Nanotechnologien

Die kontinuierliche tropfenbasierte mikrofluidische Synthese liefert Gold- und Silbernanopartikeln in verschiedenen Formen in sehr hoher Ausbeute und enger Größenverteilung. Durch Wahl der Konzentrationsverhältnisse der Reaktanden lassen sich Formen und Größen der Partikel und damit die optischen Resonanzen reproduzierbar einstellen. Untersuchungen an homogenen kolloidalen Lösungen von flachen Silberdreiecksprismen und Goldnanostäbchen zeigen, dass Größen- und Formeffekte auf die langwellige Absorptionsbande gut mit einer einfachen Beschreibung als 1-Photon-1-Elektron-Resonanz interpretiert werden können, was in Analogie zu molekularen Anregungsprozessen gesehen wird. Die langwelligen Absorptionsbanden der dimensionsreduzierten Partikel weisen auf Resonanzeigenschaften hin, die materialunabhängig sind und nur von der Partikelgeometrie bestimmt werden.

MM 63.3 Thu 12:30 IFW D

Single target sputter deposition of alloy nanoparticles with adjustable composition via gas aggregation cluster source — •Alexander Vahl[1], Julian Strobel[2], Wiebke Reichstein[1], Oleksandr Polonskyi[1], Thomas Strunskus[1], Lorenz Kienle[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Synthesis and Real Structure, Kaiserstr. 2, 24143, Kiel, Germany

Over the past decades, noble metal nanoparticles were well studied regarding their catalytic and optical properties. Recently, alloy (noble) metal nanoparticles gained increased interest for their additional degree of freedom to tailor properties like particle plasmon polaritons. In this work we present a simple approach to prepare noble metal alloy nanoparticles with good control over size and size distribution as well as composition. Employing a Haberland type single DC magnetron gas aggregation cluster source with a multicomponent target, AgAu alloy nanoparticles with tunable composition were embedded into a SiO2 matrix (pulsed reactive DC sputtering). Nanocomposite analysis (TEM, UV-vis, XPS) revealed the possibility of concentration variation of about 15% and a corresponding shift of the plasmonic absorption band by about 20nm.

MM 63.4 Thu 12:45 IFW D

Towards Graphene synthesis: a comparative study of Nickel/SiO2/Si annealing in vacuum and hydrogen — •Fatima Akhtar[1], Grzegorz Lupina[1], Peter Zaumseil[1], Sebastian Schulze[1], Andre Wolff[1], Thomas Schroeder[1,2], and Mindagaus Lukosius[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus-Senftenberg, Konrad-Zuse Straße 1, 03046 Cottbus, Germany

In microelectronics, large area growth of high quality graphene is of highest importance. Metallic catalysts like Nickel (Ni) favors the synthesis of graphene by Chemical Vapor deposition (CVD). In the present study, we show the optimization of 200 nm Ni/SiO2/Si substrates for the growth of graphene. A series of annealing was performed in the temperature range (925-1050 *C) in either vacuum or hydrogen ambient. If Ni was annealed in vacuum conditions, it was thermally stable up to 1050 *C and smoother (rms = 10.3 nm) as compared to the rms value (48.5 nm) of the samples, annealed in hydrogen atmosphere. X-ray diffraction (XRD) spectra revealed the poly-crystalline structure of Ni, where mainly Ni (111) and Ni (200) reflections have been observed. The poly-crystallinity of Ni with the main Ni (111) orientation was also confirmed by the electron back scattering diffraction (EBSD) technique. In the final step, graphene was then deposited on the annealed Ni samples, using ethylene (C2H4) as a precursor gas (deposition time: 5 min at 1x10-2 mbar pressure and deposition temperature of 925 *C). Typical G and 2D peaks were identified in the Raman spectra, indicating good quality of graphene and large grains.

MM 63.5 Thu 13:00 IFW D

Thermal and Photothermal Reshaping of Gold Nanorods — •Phillip Witthöft[1], Christian Strelow[1], Tobias Kipp[1], Gerhard Grübel[2], and Alf Mews[1] — [1]Universität Hamburg, Institut für Physikalische Chemie, Hamburg, Deutschland — [2]Deutsches Elektronen-Synchroton, Hamburg, Deutschland

Gold nanorods are cylindrical structures of colloidal gold with very interesting optical properties because of their shape dependent plasmonic resonances. The location of these plasmonic resonances in their extinction spectrum hardly depend on the aspect ratio of the nanorods. Consequently, structural changes such as melting or surface rearragement can be observed on the nanoscale following the location of the surface plasmon resonance. Here, we present different techniques to use thermal and photothermal energy to induce shape changes in gold nanorods even below the melting point. We use optical spectroscopy to track structural changes via the plasmonic resonances and compare them with transmission electron microscope images of the generated nanostructures. Based on our observation we discuss the possibilities of thermal reshaping on the nanoscale.

MM 63.6 Thu 13:15 IFW D

three dimensional image reconstruction from two dimensional image of TiO2 nanodevices — •Jesus Alan Calderon Chavarri[1], Min Zhou[2], and Yong Lei[3] — [1]TU Ilmenau, Ilmenau, Germany — [2]TU Ilmenau, Ilmenau, Germany — [3]TU Ilmenau, Ilmenau, Germany

This work describes a mathematical analysis to rebuild three dimensional (3D) image from two dimensional (2D) images of TiO2 nanodevices based on Anodic Alumina Oxide (AAO) templates, this yields to have an idea concerning part of nanodevices which can not be possible to see by figures captured by Scanning Electron Microscope SEM. For a further understanding of the mathematical analysis made in this work, it is designed simulation algorithms by MATLAB, also experiments in order to test simulation results.

MM 64: Invited talk Durst

Time: Thursday 15:00–15:30 Location: BAR 205

Invited Talk MM 64.1 Thu 15:00 BAR 205

Microstructural refinement, rate sensitivity and structural stability of Cu-X solid solutions after severe plastic deformation — •Karsten Durst — Physikalische Metallkunde, TU Darmstadt

Severe plastic deformation processes are well established for producing nanostructured and ultrafine grained metals. The influencing factors for microstructural refinement are not fully understood and are studied in this work for Cu-Al, Cu-Sn and Cu-Zn. The alloying elements have been chosen based on solid solution strengthening and stacking fault energy, where Sn is a strong solid solution strengthening element, with little influence on stacking fault energy and Zn as well as Al strongly reduce the stacking fault energy, with a medium contribution to solid solution strengthening. The mechanical properties of the alloys are assessed in both ufg and coarse-grained state using both macroscopic and nanoindentation approaches and electron back scatter diffraction in transmission mode is used to analyze the microstructural evolution. The strongest grain refinement is found for the CuSn5 alloy, which also exhibits the highest strength after severe plastic deformation. The nc-materials are highly strain rate sensitive, however CuSn5 with the lowest grain size also exhibits a low strain rate sensitivity. The paper will discuss the mechanism leading to grain refinement in conjunction with dislocation mechanism at grain boundaries, causing both a relatively low rate sensitivity and a strong refinement during SPD processing.

MM 65: Topical session: Data driven materials design - uncertainity approaches

Time: Thursday 15:45–16:30 Location: BAR 205

MM 65.1 Thu 15:45 BAR 205

Validation and uncertainty assessment of bond-order potentials for transition metals — •Matous Mrovec, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Univerität Bochum

Bond-order potentials (BOPs) present a bridge between electronic and atomistic modeling. They are based on the tight-binding (TB) approximation, but the exact diagonalization of the Hamiltonian is replaced by an approximate evaluation of the local densities of states, which leads to a real-space formalism and linear-scaling computation of the energy and forces for a system of interacting atoms. The BOP formalism can be carried out using either a numerical integration or an analytical expansion of the response functions.

In this work we present a detailed comparison of the k-space TB with the numerical and analytic BOPs for several transition metals, and assess the differences of the three approaches. The tests are carried out not only for properties of bulk phases but particular focus is given to crystal defects which are often used to validate the accuracy and reliability of interatomic potentials for transition metals.

MM 65.2 Thu 16:00 BAR 205

Numerical Quality Control for DFT–based Materials Databases — C. Carbogno[1], K. S. Thygesen[2], •B. Bieniek[1], C. Draxl[4], L. Ghiringhelli[1], A. Gulans[4], O. T. Hofmann[3], K. W. Jacobsen[2], S. Lubeck[4], J. J. Mortensen[2], M. Strange[2], E. Wruss[3], and M. Scheffler[1] — [1]FHI Berlin, Germany — [2]DTU, Lyngby, Denmark — [3]TU Graz, Austria — [4]HU Berlin, Germany

Electronic-structure theory has become an invaluable tool in materials science. Still, the precision of different approaches has only recently been scrutinized thoroughly (for the PBE functional) using extremely accurate numerical settings [1]. Little is known, however, about code- and method-specific deviances and error bars that arise under numerical settings commonly used in actual calculations. We shed light on this issue by systematically investigating the deviances in total and relative energies as function of typical settings for basis sets, **k**-grids, etc. for 71 elemental [1] and 81 binary solids in four different electronic–structure codes. On the basis of the observed trends, we propose analytical models for the estimation of error bars. They are also cross-validated using data obtained from the NoMaD Repository [2]. Eventually, we discuss the extensibility of our approach towards more complex materials properties, e.g., band gaps, and its general applicability in the context of computational materials databases.

This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Center of Excellence.
[1] K. Lejaeghere *et al.*, Science **351** (2016).
[2] *https://nomad-repository.eu*

MM 65.3 Thu 16:15 BAR 205

Sensitivity analyses for large sets of density functional theory calculations — •Jan Janssen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Over the last years methodological and computational progress in atomistic simulations has substantially improved the predictive power in materials design. However to compare the simulation results with experimental data, it is necessary to quantify the various sources of uncertainty. We therefore leverage the capabilities of our recently developed Python based workbench PyIron, to implement stochastic sensitivity analyses with the aim to differentiate model errors, statistical errors and systematical errors.

For each error we estimate the convergence gradient based on our sensitivity analyses combine it with the individual cost function of the convergence parameters and derive an algorithm for automated convergence. This approach allows us to quantify the precision not only of the energy of an individual ab initio calculation but moreover for derived quantities of sets of ab initio calculations.

MM 66: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses VI - mechanical properties

Time: Thursday 15:45–17:15 Location: IFW A

Topical Talk MM 66.1 Thu 15:45 IFW A

Molecular Dynamics Simulation On The Avalanche Dynamics and the microstructural evolution in the so called elastic region of the Cu50Zr50 — •Alexandra Lagogianni, Marius Milnikel, and Konrad Samwer — I. Physikalisches Institut, Georg-August Universität Göttingen,Göttingen,Deutschland

We present results on the study of the avalanche dynamics of a 3D Cu50Zr50 system by means of molecular dynamics simulations. The system is subjected to a finite strain rate deformation scheme and to the athermal quasistatic protocol. We find that the avalanches occur from the beginning of the so called elastic region. The critical exponents obtained by the stress drop sizes and time duration distributions for the elastic and plastic region are similar, indicating that the difference in the deformation mechanisms that govern the two regions are not depicted in these kind of statistical profiles of the avalanches. The two regions differ in the way that the number of the avalanches, their average size and the instantaneous shear modulus evolves with strain. Additionally the stress drops are accompanied by the appearance of regions in the systems that undergo shear transformations and consist of characteristic categories of clusters. The percentage of the clusters in these regions evolves upon deformation in a correlated way with the stress and the energy of the system. The overall decrease/increase of their number upon deformation is taking place by a continuous structural loop where an initial type of cluster transforms into an intermediate one of the same coordination number and consecutively this new type transforms back again to the initial state.

MM 66.2 Thu 16:15 IFW A

Mechanical properties of Palladium based bulk metallic glasses during deformation — •Niklas Nollmann, Vitalij Hieronymus-Schmidt, Isabelle Binkowski, Harald Rösner, and Gerhard Wilde — Universität Münster

Deformation of bulk metallic glasses (BMGs) at low temperatures and high stresses lead to an inhomogeneous plastic flow. During this plastic deformation the strain is localized in so called shear bands. Bulk metallic glasses show almost no ductility and fail alongside shear bands where the strain is localized. In our study we investigated PdNiP based glasses. PdNiP samples were deformed by cold rolling in several steps and the wave velocity was measured with an ultrasonic device after each step. Thus the dependence of the Poisson's ratio on the deformation state was observed. We also analyzed modifications of the mechanical properties of the metallic glass by micro alloying. Adding Iron or Cobalt to the PdNiP BMG leads to a huge change in ductility. While analyzing the dependence of the ductility of the present glasses on relaxation treatments, we utilize the fictive temperature concept to investigate the impact of minor alloying on the relative amount of free volume. Also the critical fictive temperature was measured to characterize the ductility of the new BMGs [1].

[1] G. Kumar, P. Neibecker, Y. H. Liu and J. Schroers, Nature communications 4, 1536 (2013).

MM 66.3 Thu 16:30 IFW A

microstructural fluctuations at equilibrium and under tensile deformation of a Cu-Zr model glass by molecular dynamics simulations — •pablo palomino rico[1], dimitris papageorgiou[2], and giorgos evangelakis[1] — [1]Department of Physics, University of Ioannina, Ioannina 45110 Greece — [2]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece

We present Molecular Dynamics Simulations results referring to microstructural fluctuations of a Cu65Zr35 computer glass at equilibrium and under tensile deformation. We found that at equilibrium the atoms perform short distance atomic displacements, which are not homogeneously distributed along the system, showing high and low mobility zones, and take place with the concomitance of 2 or 3 neighboring atoms, resulting in local changes of the microstructure. Inspection of the potential energy landscape of the process indicates the presence of a β-relaxation event. Under tensile deformation, those movements increase in number and distance, the high mobility zones group larger number of particles participating in such displacements and furthermore, they contribute by as much as 40% in the accommodation of the volume gain that takes place during the straining process through clusters* transformations of Icosahedra to Dodecahedra or Cuboctahedra. These results could be useful in the understanding of phenomena like aging and creep relaxation in Metallic Glasses.

MM 66.4 Thu 16:45 IFW A

Probing the mechanical properties of metallic glasses using avalanche dynamics — •Carlos Herrero-Gómez and Konrad Samwer — 1 Physikalisches Institut, Georg-August Universität Göttingen, Göttingen, Germany

Amorphous solids have been discovered, fabricated and used by mankind for more than 2000 years. Despite this fact the microscopic origin of the plasticity in such materials remain nowadays elusive. Recently such problem have been approached from the perspective of the avalanche dynamics, which allows to analyze correlations during deformation [1]. We report the avalanche analysis of several deformation experiments in metallic glasses. Based in creep tests of PdCuSi metallic glasses, we report a crossover on the deformation behavior that we associate to the strain rate [2]. In addition, we use creep tensile experiments on several amorphous materials to show that the avalanche statistics are reproduced in different systems. Finally we analyze the effect of an external magnetic field on the mechanical properties of a magnetostrictive magnetic metallic glasses, in order to study the magneto-mechanical coupling. Financial support from the ITN-FP7 Marie Curie program VitriMetTech N. 607080 is thankfully acknowledged.

Literature:

[1] Salje et al Annu. Rev. Condens. Matter Phys. 5.1 (2014): 233-254.

[2]C.Herrero-Gómez and Konrad Samwer. Scientific Reports 6 (2016).

MM 66.5 Thu 17:00 IFW A

Transformation-mediated ductility in bulk metallic glass composites — •Daniel Sopu[1], Mihai Stoica[1], and Jürgen Eckert[2] — [1]IFW Dresden, Helmholtzstr. 20, 01069, Institut für Komplexe Materialien, Dresden, Germany — [2]Erick Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, A-8700 Leoben, Austria

We investigate the influence of various critical structural aspects such as crystallite phase, size and distribution on the deformation behavior of Cu64Zr36 bulk metallic glass composites. By using molecular dynamics simulations we provide an effective strategy to control the strain localization in these composites. We show that the shear band nucleation and localization is strongly influenced by the martensitic transformation of the B2 CuZr nanocrystallites. Moreover, the martensitic transformation perturbs the local atomic strain around the nanocrystals leading to broadening of the shear bands when approaching these nanocrystals. The width increase of a shear band reduces the elastic shear stress in the vicinity of the nanoparticles, and thereby impedes the further propagation and formation of critical shear bands. This unique deformation mechanism promote ductility and work hardening in bulk metallic glass composites.

MM 67: Mechanical Properties I

Time: Thursday 15:45–16:45 Location: IFW D

MM 67.1 Thu 15:45 IFW D

On the effects of precipitates during cyclic deformation of AA6016 alloy — •Haichun Jiang, Stefanie Sandlöbes, and Sandra Korte-Kerzel — RWTH Aachen University, Aachen, Germany

Fatigue is one of the major failure modes of structural materials. While the effects of strengthening precipitates on the mechanical properties of heat treatable aluminum alloys during forming operations are well-studied, only little is known about the related mechanisms during fatigue. We study the influence of precipitates during low cycle fatigue of an Al-Si-Mg alloy by mechanical testing and microstructure characterisation using electron backscatter diffraction and scanning transmission electron microscopy (STEM). Under-aged, peak-aged and over-aged precipitation states are studied. The experiments reveal a significant influence of the precipitate state on both, the mechanical properties and the formed dislocation structures.

MM 67.2 Thu 16:00 IFW D

Surface Roughness and Deformation Avalanches — •Adam Hinkle and Lars Pastewka — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

Most natural and man-made surfaces appear to be rough on many scales. However, there is presently no unifying theory of the origin of surface roughness. One likely contributor to the formation of roughness is the process of mechanical deformation. In particular, the plasticity observed in mechanically driven amorphous solids has been characterized by avalanches of irreversible rearrangements exhibiting a self-affine, power-law behavior. Here we show preliminary results of molecular dynamics studies of metallic glasses under bi-axial compression and the resulting roughness of the free surfaces. In particular, we connect the self-affine nature of the surface roughness appearing in the power spectral density to the avalanche behavior of the deforming system.

MM 67.3 Thu 16:15 IFW D

Development and characterization of tungsten multi-fiber reinforced tungsten composites produced by field assisted sintering technology — •Yiran Mao[1], Jan Coenen[1], Johann Riesch[3], Sree Sistla[2], Bruno Jasper[1], Alexis Terra[1], Christian Linsmeier[1], and Christoph Broeckmann[2] — [1]Institut für Energie und Klimaforschung Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Institut für Werkstoffanwendungen im Maschinenbau (IWM), RWTH Aachen University, 52062 Aachen — [3]Max-Planck-Institut für Plasmaphysik, 85748 Garching b. München

In future fusion reactors, tungsten is a main candidate material for the first wall and the divertor. The intrinsic brittleness of tungsten is, however, a concern with respect to the fusion environment. To overcome this drawback, tungsten fiber reinforced tungsten (Wf/W) composites are being developed relying on an extrinsic toughing principle. Recent progress on multi-fiber Wf/W produced by field assisted sintering technology will be presented. Preliminary mechanical tests have been performed in the as-fabricated condition. A pre-notched 3-point bending test (at RT) has been chosen to observe the fracture behavior of the Wf/W. With the optimization of the interface between the fiber and matrix, the possibility to realize the pseudo ductility mechanism has been observed based on the test results. The flexural strength and tensile strength of the Wf/W have been measured by a 4-point bending test and a tensile test, respectively. The Wf/W composites with various fiber volume fractions (from 20% to 60%) have been produced and characterized, both microstructurally and mechanically.

MM 67.4 Thu 16:30 IFW D

Nanotribology and deformation behavior of gradually crystallized Fe-based metallic glasses — •Jazmin Duarte Correa, Steffen Brinckmann, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Although metallic glasses are acknowledged for their superior mechanical, physical and chemical properties, they are seldom used due to the limitations imposed by the required fast cooling rates to produce large volumes of material, and by their thermal stability. A window of opportunity is the use of these alloys at small length scales, e.g. gears for micromotors, or in wear and corrosion protective coatings.

In particular, Fe-based amorphous materials have been already proposed for both applications since they exhibit remarkable mechanical properties such as high yield stress and elastic stiffness, low strain hardening rates and low temperature dependence of the flow stress. For this work, samples of amorphous Fe-Cr-Mo-C-B alloys were gradually crystallized and submitted to nanoindentation and nanotribology tests. We discuss the correlation of the changing microstructure to the deformation behavior and the material strength. For instance, while the hardness of the alloy alloy increases with increasing crystallization, the wear resistance decreases due to the formation of a complex nanostructure formed by carbides and intermetallic phases.

MM 68: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII

Time: Thursday 16:00–18:30 Location: GER 38

Invited Talk MM 68.1 Thu 16:00 GER 38
Spectacular success of DFT in predicting novel topological phases — •Arun Bansil — Northeastern Univ, Boston USA

The revolutionary discovery of topological insulators has turned out to be the proverbial tip of the much larger iceberg of exotic phases of quantum matter driven by spin-orbit coupling effects. The consideration of electronic states protected by time-reversal, crystalline and particle-hole symmetries has led to the prediction of many novel materials that can support Weyl, Dirac and Majorana fermions, and to new types of topological crystalline and Kondo insulators, and quantum spin Hall insulators with large band gaps. The first-principles DFT-based band theory paradigm has been a key player not only in this discovery process but also in identifying salient characteristics of topological states, enabling direct and sharpened confrontation between theory and experiment. [1] I will discuss our recent theoretical work aimed at predicting topological materials and identify cases where the materials have been realized successfully. [2-10] I will also comment on the potential of topological materials as next generation platforms for manipulating spin and charge transport and other applications.

[1] Bansil, Lin and Das, Rev. Mod. Phys. 88, 021004 (2016). [2] Chang et al, Sci. Adv. 2, e1600295 (2016). [3] Huang et al., PNAS 113, 1180 (2016). [4] Zheng et al., ACS Nano 10, 1378 (2016). [5] Xu et al., Science 349, 613 (2015). [6] Zeljkovic et al., Nat. Mat. 14, 318 (2015). [7] He et al., Nat. Mat. 14, 577 (2015). [8] Xu et al., Nat. Phys. 11, 748 (2015). [9] Crisostomo et al., Nano Lett. 15, 6568 (2015). [10] Xu et al., Sci. Adv. 1, e1501092 (2015).

MM 68.2 Thu 16:30 GER 38
Interlayer excitons and Band Alignment in MoS$_2$/hBN/WSe$_2$ van der Waals Heterostructures — •Simone Latini — Technical University of Denmark, Copenhagen, Denmark

Van der Waals Heterostructures (vdWHs) are a unique platform for the realization of novel (opto)-electronic devices with embedded multi-functionality. Combining two-dimensional (2D) semiconductors with misaligned band edges can lead to the formation of photo-excited electrons and holes localized in distinct layers, which result into interlayer excitons. Understanding the energetics behind the formation of interlayer excitons is the first step towards the engineering of charge separation processes in photovoltaic devices and photodetectors. The contribution of our work is then twofold. (I) We calculate, for the first time, the interlayer exciton binding energies in complex vdWHs, specifically MoS$_2$/hBN/WSe$_2$ heterostructures, using a first-principles approach. The binding energy is of extreme technological importance as it is a measure of how strongly the electron-hole pair is bound and hence how easily it can be separated. (II) We obtain accurate electronic band edges at the interface between the layers of the vdWHs, a task which could not yet be accomplished with any available state of the art technique. Importantly, the accuracy of our calculated exciton binding energies and band edges is confirmed by a striking agreement with experimental data on photoluminesce of interlayer excitons in MoS$_2$/hBN/WSe$_2$ heterostructures.

MM 68.3 Thu 16:45 GER 38
Trionic effects in graphene nanoribbons and further nanomaterials — •Thorsten Deilmann and Kristian Sommer Thygesen — Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Among low-dimensional materials armchair-edged graphene nanoribbons are very promising candidates with optical properties which are dominates by excitons. In the presence of additional charges, trions (i.e. charged excitons) can occur in the optical spectrum. With our recently developed first-principle many-body approach [1], we predict strongly bound trions in nanoribbons with decreasing binding energies of 660 to 140 meV for widths of 3.6 to 14.6 Å. We determine their optical spectra and identify several trions by their real-space wave functions. [1] Phys. Rev. Lett. **116**, 196084.

MM 68.4 Thu 17:00 GER 38
Interface Structure Prediction using the Ab Initio Random Structure Searching Method — •Georg Schusteritsch and Chris Pickard — Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, U.K.

First-principles structure prediction of bulk materials is now routinely performed, however the field of predicting the atomic structure of interfaces is still in its infancy. A detailed understanding of and ability to predict the atomic structure of interfaces is however of crucial importance for many technologies. Interfaces are very hard to predict due to the complicated geometries, crystal orientations and possible non-stoichiometric conditions involved and provide a major challenge to structure prediction. We present here the ab initio random structure searching (AIRSS) method and how it can be used to predict the structure of interfaces. Our method relies on generating random structures in the vicinity of the interface and relaxing them within the framework of density functional theory. The method is simple, requiring only a small set of parameters, and can be efficiently run on modern parallel computer architectures. We focus here on the prediction of grain boundaries, but application to heterostructure interfaces is straightforward. Examples for several grain boundary defects in technologically important materials will be presented: In particular grain boundaries in graphene, the prototypical two-dimensional material will be discussed, alongside with examples of grain boundaries in transition metal oxides, such as SrTiO3 and TiO2.

MM 68.5 Thu 17:15 GER 38
Predicting new materials and their properties with supercomputers: the example of perovskites — •Silvana Botti[1] and Miguel A.L. Marques[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Can new materials with optimized properties be designed using supercomputers?

I will try to convince you through the example of the search of new perovskites that first-principles calculations can efficiently speed up the discovery of new materials.

Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, and are therefore suitable tools for understanding the physics not only of simple perfect crystals, but also of nanostructured materials, doped semiconductors, interfaces, alloys, etc. As a result, ab initio simulations of spectroscopic properties can finally account for the complexity of "real" experimental samples, allowing accurate comparison of calculated and measured structural and excitation properties. The powerful combination of theoretical spectroscopy with high-throughput calculations, structural prediction and machine learning can therefore provide a precious guide to experimentalists in the search of new materials.

MM 68.6 Thu 17:30 GER 38
Spectral property prediction with artificial neural networks — •Annika Stuke[1], Milica Todorovic[1], Kunal Ghosh[2], Aki Vehtari[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]Helsinki Institute of Information Technology, Department of Computer Science, Aalto University, Finland

The ability to efficiently design new and advanced optoelectronic materials is hampered by the lack of suitable methods to rapidly and accurately identify yet-to-be-synthesized materials that meet a desired application. To overcome such design challenges, a machine learning model based on a deep multi-task artificial neural network (ANN) is presented that can predict spectral properties of small organic molecules. The ANN is trained and validated on data generated by accurate state-of-the art quantum chemistry computations for diverse subsets of the GDB-13 and GDB-17 datasets [1,2]. The molecules are represented by a simple, easily attainable numerical description based on nuclear charges and cartesian coordinates and are mapped onto multiple excited-state properties simultaneously using a deep ANN trained by gradient descent and error backpropagation [3]. This on-demand prediction model can be used to infer spectral properties of various candidate molecules in an early screening stage for new optoelectronic materials at negligible computational cost, thereby completely bypassing conventional laborious approaches towards materials discovery.

[1] L. C. Blum et al., J. Am. Chem. Soc. 2009, 131, 8732, [2] R. Ramakrishnan et al., Scientific Data 2014, 1, 140022, [3] G. Montavon et al., New J. Phys. 2013, 15, 095003

MM 68.7 Thu 17:45 GER 38

Machine-Learning Based Interatomic Potential for Amorphous Carbon — •Volker Deringer and Gábor Csányi — University of Cambridge, Cambridge, UK

Machine-learning based interatomic potentials are currently of growing interest in the solid-state theory communities, as they enable materials simulations with close-to DFT accuracy but at much lower computational cost. Here, we present such an interatomic Gaussian approximation potential (GAP) model for liquid and amorphous carbon. We first discuss the maximum accuracy that any finite-range potential can achieve in carbon structures; then, we show how a hierarchical set of two-, three-, and many-body structural descriptors can be used to fit a GAP that indeed reaches the target accuracy. The new potential yields accurate energetic and structural properties over a wide range of densities; it also correctly captures the structure of the liquid phases, at variance with state-of-the-art empirical potentials. Exemplary applications to surfaces of "diamond-like" tetrahedral amorphous carbon (ta-C) will be presented, including simulations of high-temperature surface reconstructions ("graphitization"). The method appears to be promising for realistic and accurate simulations of nanoscale amorphous carbon structures.

MM 68.8 Thu 18:00 GER 38

High-throughput computational search for new high mobility transparent (semi)conducting materials — •Geoffroy Hautier[1], Joel Varley[2], Anna Miglio[1], David Waroquiers[1], Viet-Anh Ha[1], and Gian-Marco Rignanese[1] — [1]Université catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Lawrence Livermore National Laboratory

Transparent conducting oxides (TCMs) are large band gap materials (to favor transparency) doped with electrons (n-type) or holes (p-type). TCMs are essential to many technologies from solar cell to transparent electronics and there is currently a large effort towards the discovery of new TCMs. I will present the results of a high-throughput computational search for new TCMs especially directed at p-type materials. Focusing on low effective masses (leading to high mobility), large band gaps and dopability, I will show how thousands of compounds can be screened using various ab initio techniques (from density functional theory to GW) to find new potential high performance TCMs. I will discuss several unsuspected compounds with promising electronic structures and when available link our findings to experimental results. Beyond the description of those novel TCM candidates, I will chemically rationalize our findings, highlighting several design strategies towards the development of future high mobility TCMs.

MM 68.9 Thu 18:15 GER 38

Cross-validation in the cluster expansion method — •Axel Hübner, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

The cluster expansion technique allows the construction of model Hamiltonians for an efficient evaluation of the total energy of alloys. This technique relies on a fit to a small set of *ab-initio* calculations for selected atomic configurations. Key aspects to maximize the predictive performance of the model are the selection of a set of basis functions, i.e. clusters, and of configurations. To achieve this, the cross-validation technique is typically used [1]. In this work, an analytical formula for the calculation of the leave-many-out cross-validation score (CV) is derived. This formula exhibits numerical instabilities, whose analytical properties yield a criterion for structure selection in cluster expansions. Moreover, a relation between the noise in the data and the CV is outlined. This leads to a tool which allows us to estimate, for a given noise level, the size of the ab-initio data set upon which no improvements of the model are obtained. These results are exemplified for a cluster expansion of the thermoelectric clathrate alloy $\mathrm{Ba_8Al}_x\mathrm{Si}_{46-x}$, calculated with the `CELL` package [2].

[1] A. van d. Walle *et al.*, Journal of Phase Equilibria 23 (2002), Aug., Nr. 4

[2] M. Troppenz *et al.*, submitted (2016); S. Rigamonti *et al.*, in preparation.

MM 69: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses VII - thermodynamics and structure

Time: Thursday 17:30–19:00 Location: IFW A

MM 69.1 Thu 17:30 IFW A

Vibrating-reed mechanical spectroscopy of an electrodeposited Ni-P nanoglass — •Hans-Rainer Sinning[1], Yulia Ivanisenko[2], Tao Feng[3], Di Wang[2], Herbert Gleiter[2,3], and Horst Hahn[2,3] — [1]Institut für Werkstoffe, Technische Universität Braunschweig, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]Herbert Gleiter Institute of Nanoscience, Nanjing University of Science and Technology, China

A nanoglass with a composition near $\mathrm{Ni_{83}P_{17}}$ consisting of nanometer-sized amorphous "grains" and amorphous interfaces between these grains was prepared by a multi-phase pulse electrodeposition technique. As-deposited films were cut into 1mm x 10mm stripes and studied by mechanical spectroscopy at frequencies between 0.1 and 3 kHz using the vibrating-reed technique. Temperature-dependent spectra of internal friction and elastic stiffness were measured between 100 and 800 K. A thermally activated relaxation peak was observed above 400 K, followed by some irreversible transformation around 500 K after which the relaxation peak disappears. This transformation prevents an accurate determination of the activation parameters, which can only roughly be estimated to be of the order of 1 eV and 10^{13} s^{-1}. The relaxation may be discussed from different viewpoints either as a type of beta relaxation, or as an interface relaxation somehow analogous to grain boundary relaxation in polycrystals. A final crystallization effect was found in both elastic modulus and internal friction at 750 K, which is 150 K higher than the crystallization of a conventional, melt-spun Ni-P metallic glass.

MM 69.2 Thu 17:45 IFW A

Cryogenic Rejuvenation of Metallic Glasses — •Jonas Lübke, Isabelle Binkowski, Niklas Nollmann, Martin Peterlechner, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Germany

The material class of metallic glasses shows interesting properties such as high strength, toughness and corrosion resistance. However, a severe lack of ductility makes the material unsuitable for many applications. In the past, a lot of work was concentrated on reducing this disadvantage using micro-alloying or crystalline precipitates with notable success. A different approach is the concept of ”free volume” in metallic glasses. The redistribution of present free volume may lead to enhanced ductility. This so called rejuvenation can be achieved by mechanical preloading in the elastic regime. Ketov et al. [1] claim to achieve this rejuvenation by using the heterogeneous thermal expansion coefficient of metallic glasses to induce internal strain by thermal cycling. To avoid structural relaxation these cycles have to be at cryogenic temperatures. By this the ductility of the metallic glass is said to be improved in a different and simple way. In this contribution effects of different degrees of cryogenic rejuvenation, i.e. change in cycle numbers and resting times at different temperatures, on the metallic

glasses Vitreloy1, $Pd_{40}Ni_{40}P_{20}$ and $Pd_{39}Ni_{41}P_{20}$ on their amount of free-volume, structural relaxation and mechanical properties are presented and discussed.
[1] S. V. Ketov et al. Rejuvenation of metallic glasses by non-affine thermal strain. Nature 524, 2015

MM 69.3 Thu 18:00 IFW A

Effect of Co microalloying on the low-temperature heat capacity of $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass — •Rene Hubek[1], Mikhail Seleznev[2], Isabelle Binkowski[1], Martin Peterlechner[1], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Togliatty State University, Togliatty, Russia

The physical properties of bulk metallic glasses are a subject of intensive research especially with respect to their mechanical behavior. Recently it was shown that the mechanical properties of a model $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass could significantly be enhanced through cobalt microalloying [1]. The present study is focused on the impact of the microalloying on the low-temperature heat capacity. The results are discussed in comparison to the heat capacity data of a reference $Pd_{40}Ni_{40}P_{20}$ glass, specifically concerning the impact of microalloying on the excess heat capacity at low temperatures that is known as "boson peak" and concerning its specific response on plastic deformation [2]. An additional magnetic heat capacity anomaly is observed in the low temperature region of Co-alloyed $Pd_{40}Ni_{40}P_{20}$ glass. The effect of annealing on low-temperature heat capacities of as-cast and cold-rolled glasses is carefully analyzed.

[1] N. Nollmann et al., Scripta Mareriala 111 (2016), 119-122
[2] Yu. Mitrofanov et al., Phys. Review Letters 112 (2014)

MM 69.4 Thu 18:15 IFW A

Characterization of the Fe67Mo6Ni3.5Cr3.5P12C5.5B2.5 bulk metallic glass forming alloy — •Benedikt Bochtler, Oliver Gross, Isabella Gallino, and Ralf Busch — Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany

The bulk metallic glass steel Fe67Mo6Ni3.5Cr3.5P12C5.5B2.5 is characterized in detail to evaluate its general applicability [1]. This alloy was designed by Johnson et al. [2] and provides a high critical casting thickness of 13 mm. For the casting of amorphous parts, as well as the processing via thermoplastic forming, thermodynamics and viscosity of an alloy are crucial. The thermophysical properties, including the specific heat capacity, were measured using calorimetric methods. The crystallization behavior of amorphous samples upon heating was characterized by DSC and XRD and a TTT diagram was constructed. The equilibrium viscosity below the glass transition as well as volume relaxation behavior were measured by three-point beam bending and dilatometry, to assess the kinetic fragility. Viscosity in the liquid state was determined, using electromagnetic levitation in microgravity on a reduced gravity aircraft. The alloy displays a strong liquid behavior at low temperatures and a fragile behavior at high temperatures. These results are analog to the ones observed in several Zr-based bulk metallic glass forming liquids [3], indicating a strong to fragile liquid-liquid transition. Ref.: [1] B. Bochtler, et al., Acta Materialia, 118: 129-139, (2016) [2] J.H. Na, et al., US Patent App. 14/335,163; #20150020929 A1, (2015) [3] S. Wei, et al., Nature Comm, 4: 2083, (2013)

MM 69.5 Thu 18:30 IFW A

Thermodynamic and dynamic studies of phosphorus containing bulk glass forming liquids — •Oliver Gross, Benedikt Bochtler, Moritz Stolpe, Simon Hechler, William Hembree, Ralf Busch, and Isabella Gallino — Saarland University, Chair of Metallic Materials, Campus C6.3 66123 Saarbruecken, Germany

Phosphorous containing bulk metallic glass forming alloys (BMGs) are among the best metallic glass formers known to date. The newly developed Ni-P-based BMGs are no exception (critical casting thickness *1 cm) and provide an attractive alternative to Zr-based BMGs for industrial applications due to their relatively inexpensive constituents, good processability and exceptional corrosion resistance. Pt-P-based BMGs feature a large supercooled liquid region and an attractive color, which makes them highly promising for jewelry applications.

In this comparative study, the thermophysical properties of different phosphorus containing alloys (Ni-P, Pt-P) are investigated using differential-scanning calorimetry and thermal mechanical analysis for the determination of the specific heat capacity and equilibrium viscosity, respectively. The specific heat capacity data was used to calculate the enthalpy and entropy difference between the liquid and the crystalline mixture. Interestingly, the alloys differ considerably in their thermodynamic properties, whereas they show a similar behavior in the temperature dependence of their equilibrium viscosity.

MM 69.6 Thu 18:45 IFW A

Thermodynamic and kinetic properties as well as low temperature relaxations of Mg-based bulk metallic glasses — •Maximilian Frey, Ralf Busch, and Isabella Gallino — Chair of Metallic Materials, Saarland University

A broad set of thermodynamic and kinetic properties of four Mg-based metallic glass forming systems was established using calorimetric studies, thermophysical analysis, as well as thermomechanical analysis. Beside considerations about the fragilities of these alloys, especially the appearance of a secondary relaxation event occuring at temperatures distinctly below the glass transition was analysed via modulated DSC scans and isochronal DMA measurements. The definition of the Johari-Goldstein-type secondary relaxation as a general feature of metallic glasses has become increasingly popular in recent literature. However, the present relaxation signals exhibit characteristics, which are atypical for this kind of secondary event, like e.g. relatively high activation energies of about 135 kJ/g-atom. In combination and consistency with other works also investigating a Mg-based alloy via DMA and XPCS, a model is presented that explains the secondary relaxation event through a broad structural relaxation time spectrum. In this light, the corresponding measurement signals are interpreted as the premature thawing of defect regions, which exhibit increased free volume and are embedded in the surrounding more densely packed glassy backbone.

MM 70: Mechanical Properties II

Time: Thursday 17:00–18:15 Location: IFW D

MM 70.1 Thu 17:00 IFW D

The Origin of Microstructural Discontinuities underneath a Tribologically Loaded Surface — •Christian Greiner[1], Zhilong Liu[1], Reinhard Schneider[1], Lars Pastewka[1], and Peter Gumbsch[1,2] — [1]KIT, Kaiserstrasse 12, 76131 Karlsruhe — [2]Fraunhofer Institute for Mechanics of Materials IWM, Woehlerstrasse 12, 79108 Freiburg, Germany

Frictional loading of a metal surface induces microstructural changes underneath the surface. A typical tribo-induced microstructure displays distinct discontinuities parallel to the surface which separate the near surface layer from the bulk. By systematically decreasing the number of passes of a sapphire sphere sliding over high-purity copper, we find that the origin of the microstructural discontinuity is already laid after the first sliding pass even for very mild sliding conditions. A distinct dislocation structure is formed 100-150 nm under the surface. This distinct dislocation self-organization is attributed to a sign change in the stress field underneath the sliding indenter. The dislocation structure evolves into the known microstructural features with increasing number of sliding passes. Consequently, the microstructure and mechanical properties of the surface layer are determined in the very first loading pass. Control of the initial tribological loading could therefore be exploited to precondition interfaces for superior tribological properties.

MM 70.2 Thu 17:15 IFW D

Towards understanding fracture toughness experiments at the microscale — •Steffen Brinckmann and Gerhard Dehm — Max-Planck-Institut für Eisenforschung

Micrometer cantilever beams are frequently employed to determine the fracture toughness of (1) single phases in poly-phase materials as well as (2) particular grain boundaries. The determination of the mechanical properties mostly relies on the experimentally determined maximum force and analytical models which are build for brittle and isotropic materials. However, the vast majority of materials has a limited amount of plasticity and is anisotropic. Moreover, the cantilever width has an influence on the fracture toughness since the crack driving force is maximal in the beam center and plane-stress conditions apply at the beam surface. This contribution uses the results of more than a thousand 3D simulations and quantifies the influence of anisotropy, Poisson's ratio and beam geometry. At the end of the contribution, we discuss the influence of plasticity and its challenges. We give best-practice guidelines for microbeams and discuss the changes in fracture toughness, if guidelines cannot be fulfilled or if anisotropic materials are studied.

MM 70.3 Thu 17:30 IFW D

Hydrogen embrittlement of tungsten using deuterium plasma charging and microscale fracture experiments — •Xufei Fang[1], Marcin Rasinski[2], Arkadi Kreter[2], Dmitry Matveev[2], Rafael Soler[1], Steffen Brinckmann[1], Christoph Kirchlechner[1], Christian Linsmeier[2], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany — [2]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung-Plasmaphysik, 52425 Jülich, Germany

Hydrogen embrittlement (HE) is the cause of widespread failure of engineering structures. In this work we report fracture toughness and indentation experiments to study the HE of tungsten. Micro-cantilevers with pre-notches were cut using a Focus Ion Beam into single large grains that were selected by using Electron Backscatter Diffraction. The samples with micro-cantilevers were charged with deuterium plasma (max ion flux 5.0E+21 m-2s-1) and were mechanically investigated. Micro-cantilever fracture experiments at different times (i.e. 5h, 24h, 72h) after plasma charging were carried out and compared to those of uncharged micro-cantilevers. Load-displacement curves and post-mortem scanning electron microscopy showed that both charged and uncharged cantilevers exhibit plastic deformation and a blunted crack tip with a trace of crack tip sharpening. We will discuss these findings, the evolution of the unloading-reloading stiffness and correlate them to the nanoindentation results to shed more light on the hydrogen effect on the mechanical properties of tungsten.

MM 70.4 Thu 17:45 IFW D

Microstructure evolution in pearlite during microscale wear experiments — •Caroline Fink, Steffen Brinckmann, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

We study friction and wear of a microasperity on a smooth surface to enhance the understanding of macroscopic friction. This study focuses especially on the tribologically induced microstructure evolution in pearlitic steel. The bulk pearlite is mechanically ground and polished to achieve a flat surface. Single microscratches are performed by a conical diamond tip of a few micrometer radius in a nanoindenter. After target preparation, the microstructure underneath the scratch is studied with scanning electron microscopy. We observed matrix grain refinement, lamellae fracture and bending. We further investigate the latter with cementite fracture toughness and bending experiments by using microcantilevers inside an in-situ nanoindenter. Furthermore we evaluate tribological surface layer formation via electron backscatter diffraction.

MM 70.5 Thu 18:00 IFW D

Rupture of graphene sheets with randomly distributed defects — •Samaneh Nasiri and Michael Zaiser — Department of Materials Science and Engineering, WW8-Materials Simulation, Friedrich- Alexander University Erlangen-Nürnberg, Fürth, Germany

We use atomistic simulation (molecular mechanics and molecular dynamics) to investigate failure of graphene sheets containing randomly distributed vacancies. We investigate the dependency of the failure stress on defect concentration and sheet size and show that our findings are consistent with the Duxbury-Leath-Beale (DLB) theory of mechanical or electric breakdown in random media. The corresponding distribution of failure stresses falls into the Gumbel, rather than the Weibull class of extremal statistics. By comparing molecular mechanics and zero-temperature molecular dynamics simulations we establish the role of kinetic energy in crack propagation and its impact on crack patterns emerging before sheet rupture.

Keywords: graphene; fracture; microcracks; disordered media; extremal statistics

MM 71: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Time: Friday 10:30–13:00 Location: HSZ 02

Invited Talk MM 71.1 Fri 10:30 HSZ 02

Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — •Weitao Yang — Duke University

Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. We developed a scaling correction scheme by imposing the Perdew-Parr-Levy- Balduz linearity condition. Our novel scheme leads to the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. Within many-electron theory, we have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.

Invited Talk MM 71.2 Fri 11:00 HSZ 02

Multi-reference density functional theory — •Andreas Savin — Laboratoire de Chimie Théorique, CNRS and UPMC, Univ. Paris VI, Sorbonne University, Paris, France

It is sometimes said that there is no multi-reference density functional theory. The talk presents a personal viewpoint, and will focus on the following points. 1) There are many ways to introduce multi-determinant wave functions into density functional theory. 2) Several variants have been successfully explored. 3) Difficulties inherent to approximations (both for wave functions and density functionals) persist, but can be attenuated.

Invited Talk MM 71.3 Fri 11:30 HSZ 02

Density functionals from machine learning — •Kieron Burke — UC Irvine

Machine learning is spreading to all aspects of our lives. A particular method, kernel ridge regression, has proven very useful for fitting and interpolating in high-dimensional spaces.

Several years ago, in collaboration with the group of Klaus-Robert Muller in computer science at TU Berlin, we demonstrated how to construct a machine-learned density functional on a simple toy problem, non-interacting fermions in a box. We showed both its successes and limitations. We have continued to develop this method (PRL, 2012).

I will report on two recent works. In the first (arXiv:1609.02815), we construct the non-interacting kinetic energy functional for small molecules in 3D using a basis. We avoid the challenge of finding functional derivatives by learning the potential to density map directly, thereby bypassing the need to solve the Kohn-Sham equations.

In the second, we learn the interacting functional directly for the first time. In 1D, we model chains of H atoms of different length, and learn F[n] itself, from highly accurate DMRG calculations. With a novel choice of basis for the densities, we are able to learn the functional to chemical accuracy in the thermodynamic limit (arXiv:1609.03705).

Invited Talk MM 71.4 Fri 12:00 HSZ 02

Taming Memory-Dependence in Time-Dependent Density Functional Theory — •Neepa Maitra — Hunter College of the City University of New York

The exact exchange-correlation functional of time-dependent density functional theory (TDDFT) is known to depend on the history of the densities and the initial states, a dependence which is ignored in almost all of the calculations today that use an adiabatic approximation. The lack of this dependence can sometimes lead to drastically incorrect predictions of the dynamics, as has been shown in several examples recently. We present here a new approach to developing functional approximations that breaks free of the adiabatic approximation, and test the resulting approximations on a number of model systems.

Invited Talk MM 71.5 Fri 12:30 HSZ 02

Quantum Embedding Theories — •Fred Manby — School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK

Issues of accuracy in density functional theory can be addressed by making more accurate methods (like coupled-cluster theory) more efficient; or by making density functional approximations more accurate. Efforts in both directions are underway in our group, but in this talk I will focus on a third possibility, namely the development of quantum-mechnical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.