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

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Overview of Invited Talks and Sessions

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

Invited Talks

MM 1.1	Mon	9:30–10:00	BAR 205	**Atomic resolution observations of grain boundary phase transformations** — •Christian Liebscher, Thorsten Meiners, Nicolas Peter, Timofey Frolov, Robert Rudd, Gerhard Dehm
MM 10.1	Mon	15:00–15:30	BAR 205	**High-Entropy Alloys: Materials design in high dimensional chemical space from ab initio thermodynamics** — •Fritz Körmann
MM 19.1	Tue	9:30–10:00	BAR 205	**Ultrafast calorimetry: studying phase transitions in slow motion** — •Jörg F. Löffler
MM 31.1	Wed	9:30–10:00	BAR 205	**Importance of Dislocation Character Angle and Local Stress State Dependent Mobility Laws on Discrete Dislocation Dynamics Modeling of Plasticity in Aluminum** — •Douglas Spearot, Khanh Dang, Darshan Bamney, Laurent Capolungo
MM 38.1	Wed	15:00–15:30	BAR 205	**Single Crystals of Alloys by Additive Manufacturing** — •Carolin Körner, Markus Ramsperger, Julian Pistor, Johannes Köpf, Matthias Markl
MM 48.1	Thu	9:30–10:00	BAR 205	**Molecular dynamics simulations of pressure induced phase transformations in iron and iron-carbon: Interplay of defects and phase transition** — •Nina Gunkelmann, Hoang-Thien Luu, Ramon J. Ravelo, Timothy C. Germann, Eduardo M. Bringa, Herbert M. Urbassek
MM 57.1	Thu	15:00–15:30	BAR 205	**Deformation mechanisms in metals under a tribological load** — •Christian Greiner

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYBD

See SYBD for the full program of the symposium.

SYBD 1.1	Tue	9:30–10:00	HSZ 02	**Materials innovation driven by data and knowledge systems** — •Surya Kalidindi
SYBD 1.2	Tue	10:00–10:30	HSZ 02	**Network Theory Meets Materials Science** — •Chris Wolverton, Murat Aykol, Vinay Hegde
SYBD 1.3	Tue	10:30–11:00	HSZ 02	**Verification and error estimates for ab initio data** — •Claudia Draxl
SYBD 1.4	Tue	11:15–11:45	HSZ 02	**Identifying Domains of Applicability of Machine Learning Models for Materials Science** — •Mario Boley, Christopher Sutton, Luca M. Ghiringhelli, Matthias Rupp, Jilles Vreeken, Matthias Scheffler
SYBD 1.5	Tue	11:45–12:15	HSZ 02	**Deep learning of low-dimensional latent space molecular simulators** — •Andrew Ferguson

Invited talks of the joint symposium SYED

See SYED for the full program of the symposium.

SYED 1.1	Thu	9:30–10:00	HSZ 01	**Ultrafast electron dynamics at laser-irradiated surfaces** — •Baerbel Rethfeld
SYED 1.2	Thu	10:00–10:30	HSZ 01	**Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases** — •Bradley Siwick, Martin Otto, Jan-Hendrik Pohls, Laurent Rene de Cotret, Mark Sutton
SYED 1.3	Thu	10:30–11:00	HSZ 01	**Light MATTERs!!!** — •Hrvoje Petek, Andi Li, Zehua Wang, Marcel Reutzel
SYED 1.4	Thu	11:15–11:45	HSZ 01	**Quantum localization and delocalization of charge carriers in molecular organic crystals** — •Jochen Blumberger
SYED 1.5	Thu	11:45–12:15	HSZ 01	**Single-Atom Catalysis (SAC): How Structure Influences Reactivity** — •Gareth Parkinson

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Sessions

MM 1.1–1.1	Mon	9:30–10:00	BAR 205	**Invited talk Liebscher**
MM 2.1–2.4	Mon	10:15–11:30	BAR 205	**Topical Session: Data Driven Materials Science - Materials Design I (joint session MM/CPP)**
MM 3.1–3.5	Mon	10:15–11:30	IFW A	**Transport - Atoms and Ions I**

MM 4.1–4.5	Mon	10:15–11:30	IFW B	**Microstructure and Phase Transformations - Characterization**
MM 5.1–5.5	Mon	10:15–11:30	IFW D	**Liquid and Amorphous Metals - Kinetics and Modelling**
MM 6.1–6.5	Mon	11:45–13:00	BAR 205	**Topical Session: Data Driven Materials Science - Materials Design II (joint session MM/CPP)**
MM 7.1–7.5	Mon	11:45–13:00	IFW A	**Transport - Atoms and Ions II**
MM 8.1–8.5	Mon	11:45–13:00	IFW B	**Microstructure and Phase Transformations - Processing**
MM 9.1–9.5	Mon	11:45–13:00	IFW D	**Liquid and Amorphous Metals - Brittle-to-ductile Transition**
MM 10.1–10.1	Mon	15:00–15:30	BAR 205	**Invited talk Körmann**
MM 11.1–11.3	Mon	15:45–16:45	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning for Damage Prediction**
MM 12.1–12.4	Mon	15:45–16:45	IFW A	**Transport - High Entropy Alloys**
MM 13.1–13.4	Mon	15:45–16:45	IFW B	**Microstructure and Phase Transformations - Processing and Imaging**
MM 14.1–14.4	Mon	15:45–16:45	IFW D	**Computational Materials Modelling - Methods I**
MM 15.1–15.1	Mon	17:00–17:30	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning for Production (joint session MM/CPP)**
MM 16.1–16.4	Mon	17:00–18:00	IFW A	**Transport - Heat Transport and Thermoelectricity**
MM 17.1–17.3	Mon	17:00–17:45	IFW D	**Computational Materials Modelling - Methods II**
MM 18.1–18.43	Mon	18:15–20:00	P4	**Poster Session I**
MM 19.1–19.1	Tue	9:30–10:00	BAR 205	**Invited talk Löffler**
MM 20.1–20.4	Tue	10:15–11:30	IFW A	**Topical Session: Interface-dominated phenomena - Diffusion**
MM 21.1–21.5	Tue	10:15–11:30	IFW B	**Transport - Ions and Electrons**
MM 22.1–22.5	Tue	10:15–11:30	IFW D	**Liquid and Amorphous Metals - Metallic Glass**
MM 23.1–23.5	Tue	11:45–13:00	IFW A	**Topical Session: Interface-dominated phenomena - Interactions at Interfaces**
MM 24.1–24.5	Tue	11:45–13:00	IFW B	**Materials for Sensors and Actuators**
MM 25.1–25.5	Tue	11:45–13:00	IFW D	**Liquid and Amorphous Metals - Structure**
MM 26.1–26.5	Tue	14:15–15:30	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning for Materials Properties**
MM 27.1–27.5	Tue	14:15–15:30	IFW A	**Topical Session: Interface-dominated phenomena - Nanoporous Metals**
MM 28.1–28.4	Tue	14:15–15:15	IFW B	**Computational Materials Modelling - Hydrogen in metals**
MM 29.1–29.6	Tue	14:15–15:45	IFW D	**Materials for Energy Storage and Conversion - Battery and Fuel Cell Materials (joint session MM/CPP)**
MM 30.1–30.40	Tue	18:15–20:00	P4	**Poster Session II**
MM 31.1–31.1	Wed	9:30–10:00	BAR 205	**Invited talk Spearot**
MM 32.1–32.4	Wed	10:15–11:30	BAR 205	**Topical Session: Data Driven Materials Science - Materials Data Management (joint session MM/CPP)**
MM 33.1–33.5	Wed	10:15–11:30	IFW A	**Topical Session: Interface-dominated phenomena - Hydrogen at Interfaces**
MM 34.1–34.4	Wed	10:15–11:15	IFW D	**Computational Materials Modelling - Matter-Particle Interaction**
MM 35.1–35.6	Wed	11:45–13:15	BAR 205	**Topical Session: Data Driven Materials Science - Descriptors (joint session MM/CPP)**
MM 36.1–36.4	Wed	11:45–13:00	IFW A	**Topical Session: Interface-dominated phenomena - Theoretical Approaches**
MM 37.1–37.5	Wed	11:45–13:00	IFW D	**Materials for Energy Storage and Conversion - Structure of Battery Materials**
MM 38.1–38.1	Wed	15:00–15:30	BAR 205	**Invited talk Körner**
MM 39.1–39.5	Wed	15:45–17:00	BAR 205	**Computational Materials Modelling - Alloys I**
MM 40.1–40.4	Wed	15:45–17:00	IFW A	**Topical Session: Interface-dominated phenomena - Solutes at Interfaces I**
MM 41.1–41.5	Wed	15:45–17:00	IFW B	**Computational Materials Modelling - Solids and Molecules (joint session MM/CPP)**
MM 42.1–42.5	Wed	15:45–17:00	IFW D	**Materials for Energy Storage and Conversion - Functional Materials**
MM 43.1–43.5	Wed	17:15–18:30	BAR 205	**Computational Materials Modelling - Alloys II**
MM 44.1–44.5	Wed	17:15–18:30	IFW A	**Topical Session: Interface-dominated phenomena - Solutes at Interfaces II**

MM 45.1–45.5	Wed	17:15–18:30	IFW B	**Computational Materials Modelling - Low dimensional systems**
MM 46.1–46.5	Wed	17:15–18:30	IFW D	**Materials for Energy Storage and Conversion - Electronic Properties**
MM 47	Wed	18:30–20:00	IFW A	**Annual General Meeting**
MM 48.1–48.1	Thu	9:30–10:00	BAR 205	**Invited talk Gunkelmann**
MM 49.1–49.5	Thu	10:15–11:30	BAR 205	**Structural Materials (Steels, light-weight materials, high-temperature materials) - I**
MM 50.1–50.4	Thu	10:15–11:30	IFW A	**Topical Session: Interface-dominated phenomena - Thermodynamics and Microstructure Evolution**
MM 51.1–51.5	Thu	10:15–11:30	IFW B	**Computational Materials Modelling - Mechanical Properties**
MM 52.1–52.5	Thu	10:15–11:30	IFW D	**Materials for Energy Storage and Conversion - Ion Diffusion**
MM 53.1–53.6	Thu	11:45–13:15	BAR 205	**Structural Materials (Steels, light-weight materials, high-temperature materials) - II**
MM 54.1–54.4	Thu	11:45–12:45	IFW A	**Topical Session: Interface-dominated phenomena - Crystallization and Microstructure Evolution**
MM 55.1–55.5	Thu	11:45–13:00	IFW B	**Computational Materials Modelling - Magnetic Materials**
MM 56.1–56.5	Thu	11:45–13:00	IFW D	**Materials for Energy Storage and Conversion - Intercalation**
MM 57.1–57.1	Thu	15:00–15:30	BAR 205	**Invited talk Greiner**
MM 58.1–58.5	Thu	15:45–17:15	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning for Materials Characterization (joint session MM/CPP)**
MM 59.1–59.6	Thu	15:45–17:15	IFW A	**Computational Materials Modelling - Potentials**
MM 60.1–60.6	Thu	15:45–17:15	IFW B	**Mechanical Properties: Plasticity, fracture, fatigue, wear - I**
MM 61.1–61.6	Thu	15:45–17:15	IFW D	**Nanomaterials - I**
MM 62.1–62.6	Thu	17:30–19:00	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning Applications (joint session MM/CPP)**
MM 63.1–63.6	Thu	17:30–19:00	IFW A	**Computational Materials Modelling - Electronic Structure of Complex Materials**
MM 64.1–64.6	Thu	17:30–19:00	IFW B	**Mechanical Properties: Plasticity, fracture, fatigue, wear - II**
MM 65.1–65.6	Thu	17:30–19:00	IFW D	**Nanomaterials - II**

Annual General Meeting of the Metal and Material Physics Division

Wednesday 18:30–20:00 IFW A

MM 1: Invited talk Liebscher

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

Invited Talk MM 1.1 Mon 9:30 BAR 205

Atomic resolution observations of grain boundary phase transformations — •Christian Liebscher[1], Thorsten Meiners[1], Nicolas Peter[1], Timofey Frolov[2], Robert Rudd[2], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Lawrence Livermore National Laboratory, Livermore, USA

The theory that grain boundaries (GBs) can undergo phase transformations has a long history. More than 50 years ago, thermodynamic concepts have been established that GBs can exist in multiple phase states. It was assumed that stable and metastable states exist for different GB orientations. Only indirect measurements have indicated the existence of interfacial transitions and the search for these GB phases has been in vain.

Here, we present atomic resolution insights into grain boundary phase transformations and how they influence the interfacial properties. We combine advanced scanning transmission electron microscopy with atomistic simulations to resolve the atomic structure of GB phases and explore their atomistic and thermodynamic properties. We will show examples how nanoscale faceting transitions can either lead to anomalous segregation behavior or are triggered by solute segregation in both semiconductors and alloys. Even in elemental copper, we observe grain boundary phase coexistance at symmetric and asymmetric GBs. Evolutionary GB search finds the same structures as in experiment and finite temperature molecular dynamics simulations explore their transformation behavior.

MM 2: Topical Session: Data Driven Materials Science - Materials Design I (joint session MM/CPP)

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

Topical Talk MM 2.1 Mon 10:15 BAR 205

Data-Mining Strategies for Understanding Strength and Failure of Materials — •Stefan Sandfeld — TU Bergakademie Freiberg, Lampadiusstr. 4, 09599 Freiberg

Experimental observations and simulation data should – in principle – help to shed light on the 'inner workings' of a physical system, say, a material or specimen. There, the 'inner workings' would be the interaction of microstructural features among themselves, with the surfaces of the specimen, with defects, or with phase boundaries, to name but a few. Both experiment and simulation, however, suffer from particular problems which in many situations makes it difficult to directly compare them or to use results from one as input or support for the other.

In this presentation, we will start by giving an overview over current attempts for integrating experiment and simulation. We will then demonstrate, on the one hand, how data science approaches might be used to access data from experiments that would be otherwise inaccessible and, on the other hand, how data science also might help to reduce the high level of abstraction inherent to most simulations. With those methods, experiment and simulation might get a little closer to each, thereby helping to understand relevant mechanisms in strength and failure from a new point of view.

MM 2.2 Mon 10:45 BAR 205

Stabilities of novel Mg-based light metal high entropy alloys — •Wernfried Mayr-Schmölzer[1], Johannes Kirschner[2], Clemens Simson[4], Christoph Eisenmenger-Sittner[2], Johannes Bernardi[3], Stefan Müller[1], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]Institute of Solid State Physics, TU Vienna — [3]USTEM, TU Vienna — [4]LKR, Austrian Institute of Technology GmbH

Compositionally Complex Alloys (CCAs) consist of four or more elements alloyed in approximately equal fractions and often crystallize in a simple crystal lattice. In many cases, their mechanical properties like structural stability or ductility exceed that of common modern alloys. Usually, they contain heavy d-Orbital metals, but investigations into low density light metal CCAs have been rare up to now due to the complex binding modes of their constituents.

We use both a Cluster Expansion approach, augmented by stochastic prescreening steps, and neural network based pair potentials to scan the large configuration space of the Mg-Al-Cu-Zn system for stable phases. The training data was generated using density functional theory calculations implemented in the VASP code. In conjunction with experiments, we find that while the introduction of Al into the brittle $MgZn_2$ hexagonal Laves phase leads to phase separation and does not improve the mechanical properties of the alloy, the addition of Cu inhibits this process and leads to the formation of a highly stable cubic phase.

MM 2.3 Mon 11:00 BAR 205

Automatic design of reversible shape changing metamaterials — Silvia Bonfanti, Francesc Font Clos, Roberto Guerra, and •Stefano Zapperi — University of Milan, Milan, Italy

We have developed a computational method to design metamaterials that perform pre-determined input/output mechanical operations. Our numerical scheme to design metamaterials combines a reinforced dynamic Monte Carlo method with finite element simulations. We performed 3D printing of selected metamaterial configurations, showing that the machine-generated solutions present effciencies far exceeding those of man-designed ones. Finally, we show that machine learning algorithms can be trained to identify efficient solutions without performing simulations. The designed metamaterial units can be exploited as the building blocks of generic metamaterial machines or other actuators with higher complexity.

This work is supported by the European Research Council through the PoC project METADESIGN. The presenting author thanks the Alexander von Humboldt foundation for the Humboldt Research Award.

MM 2.4 Mon 11:15 BAR 205

Towards Building New Zeolites with Machine Learning — •Benjamin A. Helfrecht[1], Rocio Semino[1,2], Giovanni Pireddu[1,3], Scott M. Auerbach[4], and Michele Ceriotti[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Université de Montpellier, Montpellier, France — [3]Università degli Studi di Sassari, Sassari, Italy — [4]University of Massachusetts Amherst, Amherst, Massachusetts USA

Synthesizing new zeolites, which are useful for applications like gas separation and catalysis, with specific properties is an ongoing challenge in the zeolite community. Ideally, one would like to select a handful of compatible "building blocks" from which a new zeolite with desired properties can be synthesized. In this work, we make progress toward this goal by constructing an "atlas" of local atomic environments comprising several thousand all-silica zeolites from the Deem SLC PCOD database [1] using machine learning techniques. We evaluate the utility of this atlas by examining correlations between the locations of the atomic environments in the atlas and their energy and volume contributions to their parent frameworks.

[1] R. Pophale, P. A. Cheeseman, M. W. Deem, A database of new zeolite-like materials, Phys. Chem. Chem. Phys 13(27):12407-12412, 2011.

MM 3: Transport - Atoms and Ions I

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

MM 3.1 Mon 10:15 IFW A

Influence of magnetic transformation on bulk diffusion of Mn in iron — •Vladislav Kulitckii[1], Omkar Hegde[2], Tilmann Hickel[2], Chu-Chun Fu[3], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institutfür Materialphysik, Universität Münster, Germany — [2]Max Planck Institute for Iron Research GmbH, Düsseldorf, Germany — [3]Atomic Energy and Alternative Energies Commission, Gif-sur-Yvette, France

Comparing to alinear dependencein the paramagnetic state,the Arrhenius plot ofself-diffusion in alpha-iron shows a downward curvature below the Curie temperature.The magnetic transformation-induced kink of diffusion in alpha-iron was also observed for such solutes as Co, Cr, or Ni. Here we are reporting the impact of the magnetic transition on bulk diffusion of Mn. Tracer diffusion was measured by a microtome (higher temperatures) and sputtering (low temperatures) sectioning methods using the radioactive isotope 54Mn. The experiments are performed in a wide temperature range from 773 K to 1173 K.In obvious contrast to self-diffusion, a marginal if any impact of the magnetic transition on Mn bulk diffusion is found. The Mn bulk diffusion coefficient in alpha-Fe follows an Arrhenius dependence with the pre-factor of 0.0287 m2/s and the activation enthalpy of 282.8 kJ/mol. The experimental results are compared with the DFT-based theoretical predictions.

MM 3.2 Mon 10:30 IFW A

A DFT study of the electric field dependence of atomic migration barriers in hard magnetic $L1_0$ intermetallic phases — •Oskar Till[1] and Christian Elsässer[1,2] — [1]Freiburger Materialforschungszentrum FMF, Stefan-Meier-Straße 21, 79104 Freiburg — [2]Fraunhofer IWM, Wöhlerstraße 11, 79108, Freiburg

We examine the effect of an external electric field on migration barriers of atoms near surfaces in ferromagnetic binary $L1_0$ intermetallics. Using DFT surface-slab models for various surface configurations we study hops of atoms in the vicinity of the crystal surface. We are especially interested in the transition from the disordered A1 phase to the ordered $L1_0$ phase of FeNi, a promising candidate for a rare-earth-free high performance hard magnetic material. The aims are an assessment in how far electromigration effects can be effective in processing hard magnetic materials, as well as a better understanding of electromigration in intermetallic phases. Hence we extend the scope to the $L1_0$ phases of FePt, MnAl and MnGa. These four alloys cover a wide range of thermal ordering time scales and related experimental feasibilities. The investigations are part of a joint project 'Processing magnetic materials enhanced by electric fields or currents' in the DFG SPP 1959 'Fields Matter'.

MM 3.3 Mon 10:45 IFW A

Combination of ^{7}Li-Field-Cycling and $T_{1\rho}$-NMR experiments to investigate metallic lithium and lithium solid-state ion conductors. — •Philipp Seipel, Edda Winter, and Michael Vogel — AG Vogel, Institut für Physik kondensierter Materie, TU Darmstadt

Nuclear Magnetic Resonance offers a broad range of possibilities for determining correlation times of lithium ionic motion in Li-Ion conductors in the range of 10^0 s to 10^{-10} s. One method for determining the dynamics is to measure the spin-lattice relaxation T_1, which is sensitive to dynamics on the time scale of the inverse Larmor-frequency ω. For superconducting spectrometers, this is usually in the range of $\tau \approx 10^{-9}$ s. In order to investigate slow processes, it is beneficial to measure $T_1(\omega)$ at low magnetic fields ($\omega \approx$ kHz) whereas ^{7}Li-Field-Cycling NMR is a powerful method to do so [1,2]. In these experiment, it is necessary to switch between low and high magnetic fields during the measurement to enhance the signal intensity, whereby the measurable T_1 values are limited to ≥ 1 ms by a switching time. $T_{1\rho}$ measurement is a nice method to extend the range of field cycling, because it is possible to measure $T_{1\rho}$ values down to 10^{-4} s. However sample heating can cause limitations. Using metallic lithium as a model system, this study shows that both methods compliment each other nicely and with certain limitations, can also be used to determine activation energies for Li-ionic jumps in solid-state ionic conductors.
(1)M Haaks et al., PBR, 2017, DOI:10.1103/PhysRevB.96.104301
(2)J. Gabriel et al., SSNMR, 2015, DOI:10.1016/j.ssnmr.2015.06.004

MM 3.4 Mon 11:00 IFW A

Atomistic modeling of grain boundaries and their effects on oxygen vacancies in $SrTiO_3$ — •Cong Tao[1,2], Daniel Mutter[1], Daniel F. Urban[1], and Christian Elsässer[1,3] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]IAM-CMS, Karlsruhe Institute of Technology, Straße am Forum 7, 76131 Karlsruhe, Germany — [3]Freiburger Materialforschungszentrum FMF, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

Point defects, especially oxygen vacancies, are involved in the accelerated grain growth behavior observed in strontium titanate (STO) perovskites in applied electric fields. The underlying mechanisms for the redistribution of oxygen vacancies along and across grain boundaries (GB) are not yet fully understood. In order to advance the understanding at the atomic scale, we employ classical atomistic simulations to investigate structures and properties of both the symmetric and asymmetric tilt GBs in $SrTiO_3$. To locate the energetically favored sites for oxygen vacancies, their formation energies are calculated and analyzed with respect to local electrostatic potentials in atomistic supercell models. The simulation results indicate that oxygen vacancies preferentially form in the vicinity of the GBs. In addition to formation energies, the paths for oxygen vacancies migrating from all possible sites to their nearest neighbor sites are identified and systematically analyzed. The landscapes of oxygen vacancy formation energies and migration barriers are critically discussed with respect to experimental observations, in order to elucidate the specific role of GBs in trapping oxygen vacancies in $SrTiO_3$ from both theoretical and practical viewpoints.

MM 3.5 Mon 11:15 IFW A

Mutual dependence of oxygen and vacancy diffusion in dilute iron alloys and the influence of substitutional atoms — •Xiaoshuang Wang, Jürgen Fassbender, and Matthias Posselt — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

By combination of density functional theory (DFT) and an efficient method based on Atomistic Kinetic Monte Carlo (AKMC) the mutual influence of oxygen (O) and vacancy (v) diffusion in α-Fe and the effects of substitutional atoms (Ti, Y) are studied. Both oxygen and vacancy are mobile while the substitutional atoms are assumed to be immobile. Using DFT, binding energies between oxygen and vacancy at different neighbour distances and migration barriers for oxygen in the environment of a vacancy and for vacancy in the environment of an oxygen atom are determined. The most attractive state for oxygen and vacancy was found at the 1st neighbour distance. The O-v pair at the 6th neighbour distance is unstable and therefore it is impossible to reach via oxygen/vacancy jump. The newly-found simultaneous jumps of both O and v compensate the lack of state 6. By using the data obtained by DFT as inputs, the diffusion coefficient of oxygen and of vacancy are determined for given concentration of vacancy and oxygen atoms by an AKMC-based efficient method. Additionally, oxygen and vacancy diffusion were calculated in the first stage of thermal processing of ODS steel where O, Y, and Ti is purposely introduced.

MM 4: Microstructure and Phase Transformations - Characterization

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

MM 4.1 Mon 10:15 IFW B

Spatial correlations between strengthening phases in hardenable aluminum alloys — •Viktor Wessely[1], Robin Schäublin[1], Stephan S. A. Gerstl[1,2], Stefan Pogatscher[3], Peter J. Uggowitzer[1], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Scientific Center for Optical and Electron Microscopy, ETH Zurich, 8093 Zurich, Switzerland — [3]Nonferrous Metallurgy, Montanuniversitaet Leoben, 8700 Leoben, Austria

We focus on a new generation of hardenable aluminum alloys based on the concept of high-strength Al–Sc alloys that form coherent Al$_3$X L1$_2$-structured precipitates. Suitable candidates other than Sc are rare-earth or transition metals, such as Er, Zr, Hf or Yb, which have been shown to strengthen the material while simultaneously providing improved high-temperature stability. In this study we deployed thermodynamic and kinetic modeling to design alloys and their heat treatments, with subsequent mechanical and microstructural characterization. The dispersoids form as a coherent ordered phase within the fcc matrix. Studying their evolution in Al–Mg–Zn alloys with < 1 wt.% Er and Zr, we find that the Al$_3$X dispersoid phase has a significant impact on the alloys' hardening characteristics. Detailed insights into the microstructure are obtained by a multi-scale analysis based on high-end transmission electron microscopy (TEM), atom-probe tomography (APT) and molecular dynamics (MD) simulations. A key for the rational design of multi-phase strengthened aluminum alloys lies in the spatial correlation between the dispersoids and the precipitate phase.

MM 4.2 Mon 10:30 IFW B

Analysis of the miscibility gap in Copper-Nickel with Atom Probe Tomography — •Rüya Duran and Guido Schmitz — University of Stuttgart, 70569 Stuttgart, Germany

Although Copper-Nickel alloys are commonly used in technical applications, their alloying behavior at low temperatures is still controversial. Early theoretical and indirect experimental investigations indicated that the phase diagram may contain a miscibility gap. Nevertheless, direct experimental proof is missing due to the slow kinetics at low temperatures.

In this project, the miscibility gap is determined by a direct experimental method applying Atom Probe Tomography (APT) to thin film structures. The temperature and time dependence of the segregation in Cu/Ni thin films is investigated. The quantitative evaluation was made by a cluster analysis, which determines the local atomic fraction in coarse-grained analysis cells located around each detected atom. By plotting the abundances of the concentrations (histograms), the boundary concentrations of a miscibility gap for a certain temperature are given.

At temperatures of total miscibility, the cluster analysis show deviations from binomial distribution, which can be explained by statistical fluctuations in concentration. By using a recently developed model based on the probability distribution of the local concentration, important thermodynamic parameters can be extracted, like the Gibbs free energy and the chemical potential, which also can be used to predict the critical temperature of the miscibility gap.

MM 4.3 Mon 10:45 IFW B

Investigation of irradiation damage in thin plates of Ti6Al4V via high-energy x-ray diffraction — •Tim Lengler[1,4], Dieter Lott[1], Peter Staron[1], Emad Maawad[1], Sabine Riemann[2], Andriy Ushakov[3], and Gudrid Moortgat-Pick[3,4] — [1]Institute of Material Research, Helmholtz-Zentrum Geesthacht, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Zeuthen, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [4]Universität Hamburg, Hamburg, Germany

In order to ensure stable long-term operation of the planned positron source for the International Linear Collider (ILC), candidate materials for the conversion target have to be tested. The intense electron beam at the Mainz Microtron (MAMI) injector was used for first irradiation tests on thin plates of Ti6Al4V which is a promising candidate material for the positron conversion target as well as for the exit window to the photon beam absorber. In this work, the beforehand at MAMI irradiated plates, simulating realistic irradiation impacts as expected at the ILC, were studied via high-energy synchrotron diffraction in transmission geometry at the P07 beamline at PETRA III to investigate the potential irradiation damage. Complementary, standard source x-ray diffraction measurements were carried out in reflection geometry to gain sensitivity for surface modifications. The synchrotron and x-ray studies allow us to investigate the microstructure in a non-destructive way and, in particular, to observe changes in the phase composition and the grain size distribution due to irradiation that may compromise the long-term stability of the material.

MM 4.4 Mon 11:00 IFW B

In situ X-radiography observations of thin binary metallic alloys to investigate pattern formation and growth characteristics — •Maike Becker[1], Jonathan A. Dantzig[2], Laszlo Sturz[3], Matthias Kolbe[1], and Florian Kargl[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft-und Raumfahrt, 51170 Köln, Germany — [2]Department of Mechanical Science and Engineering, University of Illinois, Urbana, IL, 61801, USA — [3]Access e.V., Intzestr. 5, 52072 Aachen, Germany

X-radiography enables the observation of the solidification process in a few hundred microns thin samples of metallic alloys in real-time. The choice of thin samples avoids a superposition of the solidification structures and exploits the X-ray contrast through a clear distinction between the solid and liquid phases. Therefore, solidification characteristics like microstructure morphologies, growth velocities or concentration changes can be determined quantitatively. These data are used to better understand the influence of important material properties on microstructure formation. For example, the anisotropy of the solid-liquid interfacial energy plays an important role in the selection of growth directions and in the selection constant of the dendrite tip (and thus influences tip radius and growth velocities). The diffusion coefficient influences the formation of higher-order dendrite arms and the interaction distance between the crystals. In this context, the experimental data is used for comparison and validation of micro- and mesoscale simulations, like phase-field and dendrite needle network models.

MM 4.5 Mon 11:15 IFW B

Atomistic investigation of the elastocaloric effect in nanoporous NiTi structures — •Arne J. Klomp and Karsten Albe — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Shape memory or superelastic alloys exhibit strong elastocaloric response and can potentially be used in solid state cooling devices. The most promising material is NiTi due to the large latent heat released during the martensitic phase transition.

By constructing nanosized open porosity foams of NiTi one can in principle strongly increase the surface to volume ratio in order to improve the heat transfer between elastocaloric medium and heat transport medium. Using classical molecular dynamics simulations the thermomechanical properties and stability of NiTi nanofoams under cyclic mechanical loading is investigated.

Our work reveals that even in complex and random nanosized structures a martensic phase transition can be triggered by uniaxial compression and thus the elastocaloric effect can be exploited for cooling applications. We further show the impact of temperature on the amount of transformed phase, accumulated damage during cyclic loading, latent heat of the phase transformation and a possible coefficient of performance. Finally, the results give implications for limits of the maximum deformation as well as speed of deformation.

MM 5: Liquid and Amorphous Metals - Kinetics and Modelling

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

MM 5.1 Mon 10:15 IFW D

Nucleation rates of crystallization of a bulk metallic glass-former — •Mark Stringe, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Crystallization plays a crucial role not only regarding the production of metallic glasses via melt quenching, but also concerning the stability of the resulting metastable systems. High scanning rates in calorimetric measurements are realized using a custom-built fast differential scanning calorimeter. With this fast scanning calorimetry (FSC), samples with a mass of the order of micrograms are measured with scanning rates up to the order of 10.000 K/s. This vast range of scanning rates enables an analysis of crystallization for different levels of undercooling. An AuCuAgSi bulk metallic glass with low melting point is analyzed. In FSC it is possible to reach cooling rates to quench a glass in-situ.

Hence, the critical cooling rate can be determined directly. Thus, using FSC it is possible to obtain large datasets of measurement cycles. Statistical variations of the undercooling of the glass-forming alloy can be extracted from these datasets. Applying a Poisson process to the stochastic nature of nucleation, the activation barriers for nucleation of the crystalline phase are determined. Low activation barriers indicate a heterogeneous nucleation mechanism for crystallization of the FSC samples.

MM 5.2 Mon 10:30 IFW D

Kinetics of nucleation in undercooled binary and glass forming alloys — •Manoel W. da Silva Pinto, Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Deutschland

The undercooling and nucleation behavior of alloys was quantitatively analyzed via a statistical analysis that describes nucleation as a nonhomogeneous Poisson process. The statistical analysis of calorimetric data, previously applied to pure metals and metalloids, was now applied to binary Cu-Ge alloys, and to two glass-forming systems: Au-Si and Pd-Ni-P. The results enable the discussion on nucleation of binary and ternary mixtures in the framework of a concentration dependency of nucleation rates and glass forming ability. The presented results suggest a change in nucleation behavior already at small concentration variations. Such variations are not considered in the current classical nucleation theory used to describe the kinetics of nuclei formation in binary mixtures or glass forming alloys.

MM 5.3 Mon 10:45 IFW D

Predicting the glass formation behavior of multi-principal element alloys — •Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

In contrast to conventional alloys, multi-principal element alloys consist of several constituents in similarly high concentrations. Examples for such alloys range from solid-solution high entropy alloys, like the Cantor alloy $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$, to metallic glasses like $Pd_{40}Ni_{40}P_{20}$ or the commercially used Vitreloy $Zr_{40}Be_{22.5}Ti_{13.8}Cu_{12.5}Ni_{10}$. Both are of interest for research and commercial applications due to their favorable mechanical and chemical properties. Guo et al. showed that there is a correlation between the values of a set of thermodynamic and structural parameters of an alloy and the phases it forms[1]. In the present work this correlation is used to predict the glass formation behavior of multi-principal element alloys by calculating the relevant parameter set. The parameters are evaluated and the deduced critical cooling rate is compared to literature values on well-known glass formers.

[1] Guo, S. and C.T. Liu, Progress in Natural Science: Materials International, 2011. **21**(6): p. 433-446.

MM 5.4 Mon 11:00 IFW D

Micro-second molecular dynamics — structural relaxation and mechanical properties of a model glass system — •Peter Derlet[1] and Robert Maass[2] — [1]Condensed Matter Theory Group, Paul Scherrer Institute, Switzerland — [2]Department of Materials Science and Engineering and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, USA

Using molecular dynamics, we study the structural relaxation of a model binary Lennard-Jones glass over time scales spanning up to several tens of microseconds. These well-relaxed samples are then deformed to study the elastic and collective plastic shear activity under simple shear for a range of strain rates spanning six orders of magnitude. It is found that at the longer time-scales of deformation, significant thermally activated mobility and relaxation occurs in both the elastic and plastic deformation regimes. These results are discussed in terms of both the known elastic robustness of bulk metallic glasses, and the correlation between local structure and local plasticity.

MM 5.5 Mon 11:15 IFW D

Ultrafast melting of antimony after fs laser excitation: experiment meets fully ab-initio simulations — •Bernd Bauerhenne[1], Sascha Epp[2], Felipe Valencia[3], and Dwayne R. J. Miller[2] — [1]Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Luruper Chaussee 149, Geb. 99, 22761 Hamburg, Germany — [3]National University of Colombia, Cra 45, Bogota, Columbia

The time-resolved Bragg peak decay of a fs-laser pulse excited 30 nm thick antimony film was measured using x-ray pulses generated from a free electron laser. To predict this measured Bragg peak decay, we derived an electronic temperature (Te) dependent interatomic potential for antimony. For this, we fitted forces and energies obtained from ab-initio MD simulations of a thin antimony film at increased Te. Furthermore, we calculated the optical properities and the Te-depend electron-phonon coupling constant for antimony ab-initio. Utilizing the Te-dependent interatomic potential, the derived optical properites and the electron-phonon coupling constant, we performed MD simulations of a laser-excited 30 nm thick antimony film containing 9072 atoms. The calculated time-dependence of the Bragg-peaks shows very dood agreement with the experiment. Antimony melts within 600 fs for the highest considered laser intensity.

MM 6: Topical Session: Data Driven Materials Science - Materials Design II (joint session MM/CPP)

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

MM 6.1 Mon 11:45 BAR 205

Versatile Bayesian deep-learning framework for crystal-structure recognition in single- and polycrystalline materials — •Andreas Leitherer, Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Physical properties of a given material are directly related to its structure. In particular, in polycrystalline materials the location and nature of grain boundaries are crucial features determining their properties. For instance, mechanical characteristics of steels are strongly influenced by grain boundaries. In this work, we propose *strided pattern matching* which is a framework using single-crystal classification to investigate polycrystals. Accessible crystal-structure identification methods are either very robust – but can treat only few classes – or include a large number of classes – but are not very robust. We use a Bayesian neural network in combination with the smooth-overlap-of-atomic-positions (SOAP) descriptor, allowing us to classify, robustly and without any predefined threshold, more than 100 prototypes including not only bulk but also two- and one-dimensional materials (e.g., fullerenes). Furthermore, we are able to quantify the uncertainty in the model predictions. As an example for polycrystal investigation, we apply our model to recognize an ordered $L1_2$ phase in a disordered fcc matrix. This serves as a model system for precipitate detection in Ni-based superalloys, which are materials used in aircraft engines.

MM 6.2 Mon 12:00 BAR 205

Parametrically Constrained Geometry Relaxations for High-Throughput Materials Science — •Maja-Olivia Lenz[1], Thomas A. R. Purcell[1], David Hicks[2], Stefano Curtarolo[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Department of Materials Science and Mechanical Engineering, Duke University, Durham, USA

Exploiting crystal symmetries is a common technique to accelerate and improve electronic-structure calculations. However, this method usually fails when the global symmetry is broken, e.g., in materials with defects. We present a relaxation scheme that uses parametric geometry constraints to allow symmetry conservation at all levels [1]. We demonstrate how it can be used to relax metastable structures that are otherwise poorly addressable. Using the example of polarons in MgO [2], we showcase the ability to relax structures with local symmetry breaking with known distortion patterns. The flexibility of our constraints is particularly useful to accelerate high-throughput searches for novel materials. A performance study on several hundreds of different materials throughout the structural space has been done using the AFLOW Library of Crystallographic Prototypes [3]. The assignment of prototypes is helpful not only to enable user-friendly searches in materials

databases like NOMAD Archive but also to describe and refine terms and concepts in a prospective materials ontology.
[1] M.-O. Lenz, *et al.*, accepted in Npj Comput. Mater. (2019).
[2] S. Kokott, *et al.*, New J. Phys. **20** (3):33023 (2018).
[3] M. J. Mehl, *et al.*, Comp. Mater. Sci. **136**, S1 (2017).

MM 6.3 Mon 12:15 BAR 205

Combining ab-initio and data-guided approaches for refractory multi-principal element alloys design — •Yury Lysogorskiy[1], Alberto Ferrari[2], and Ralf Drautz[1] — [1]AMS, ICAMS, Ruhr University Bochum, Bochum, Germany — [2]Delft University of Technology, Delft, Netherlands

Refractory multiple principal element alloys (MPEA) nominally consist of several elements of the groups IV-VI at near-equal compositions in a single crystalline bcc phase that is characterized by exceptional high-temperature mechanical properties and a very high melting point. In this work we introduce a computationally tractable and accurate method, based on first-principles calculations and alloy modelling, to predict phase stability in MPEAs at arbitrary compositions. We reconstruct the complete phase diagram of the prototypical refractory MPEAs Mo-Nb-Ta-W and detect the regions where the formation of a solid solution is favorable at a given transition temperature. We then extend the modeling of temperature dependent properties with supervised machine learning (ML) and combine these results to a ML model for Vickers hardness, trained on experimental data from literature, to identify out-of-equiatomic composition regions of lower solid-solution formation temperature and higher hardness.

MM 6.4 Mon 12:30 BAR 205

Data-Efficient Machine Learning for Crystal Structure Prediction — •Simon Wengert[1], Gábor Csányi[2], Karsten Reuter[1], and Johannes T. Margraf[1] — [1]Chair of Theoretical Chemistry, TU Munich, Germany — [2]Department of Engineering, University of Cambridge, UK

The combination of modern machine learning (ML) approaches with high-quality data from quantum mechanical (QM) calculations can yield models with an unrivalled accuracy/cost ratio. However, such methods are ultimately limited by the computational effort required to produce the reference data. In particular, reference calculations for periodic systems with many atoms can become prohibitively expensive. This trade-off is critical for crystal structure prediction. Here, a data-efficient ML approach would be highly desirable, since screening a huge space of polymorphs with small stability differences requires the assessment of a large number of trial structures with high accuracy.

In this contribution, we present tailored hybrid-ML models that allow screening a wide range of crystal candidates while adequately describing the subtle interplay between intermolecular interactions such as H-bonding and many-body dispersion effects. This is achieved by enhancing a physics-based description of long-range interactions —for which an efficient implementation is available— with a short-range ML model trained on high-quality first-principles reference data. The presented workflow is broadly applicable to different molecular systems, without the need for a single periodic calculation on the reference level of theory.

MM 6.5 Mon 12:45 BAR 205

Uncovering Anharmonicity in Material Space — •Thomas Purcell, Florian Knoop, Chuanqi Xu, Matthias Scheffler, Luca Ghiringhelli, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Identifying materials with ultra-low thermal conductivities κ is the pivotal challenge in the development of more efficient thermoelectric devices. One strategy to achieve this goal is to find materials with a high level of anharmonicity, and therefore reduced phonon lifetime and κ. To help discover such materials, we calculate the anharmonicity of materials ranging from simple binary compounds to complex perovskites using the high-throughput framework *FHI-vibes* [1]. The framework automatically generates an accurate harmonic model for a material's vibrational properties, from which we determine its anharmonicity by statistically comparing the harmonic and *ab initio* forces of thermally displaced structures. Our screening not only demonstrates that anharmonicity is more prevalent in material space than previously thought, but also shows that the developed metric strongly correlates with various thermal properties. Using classes of simple binaries as an example, we show that the anharmonicity of a material can be related to its atomic, bulk, and harmonic properties via the sure independence screening and sparsifying operator (SISSO) approach [2], thus facilitating an even more efficient screening.
[1] https://vibes.fhi-berlin.mpg.de
[2] R. Ouyang, *et al. Phys. Rev. Mat.* **2**, 083802 (2018)

MM 7: Transport - Atoms and Ions II

Time: Monday 11:45–13:00 Location: IFW A

MM 7.1 Mon 11:45 IFW A

Alloys with continuous concentration gradient: comparing experiments with DFT — •Florian Reiter[1], Martin Hoffmann[1], Alberto Marmodoro[2], Andrei Ionut Mardare[1], Cezarina Cela Mardare[1], Saeedeh Sadet Ravandi[1], Achim Walter Hassel[1], and Arthur Ernst[1] — [1]Johannes Kepler Universität, Linz, Austria — [2]Ludwig-Maximilians-Universität München

Numerical methods allow quasi continuous variation of concentration changes in solid solutions via, e.g., the coherent potential approximation in the multiple scattering theory, which is uncommon in experimental methods. By physical vapor deposition it is possible to create compositional libraries of alloy systems, which allows a comparison with continuous experimental results. For this purpose, the resistivity of an Ag-Pd alloy was measured and related with the calculated Fermi surface. The latter can be obtained from the Bloch spectral function evaluated at the Fermi energy. The calculated Fermi surface shows a significant conformance with the expected nonlinear changes in the experimental resistivity data and can hence be considered representative for the electronic structure of the Ag-Pd alloy. In addition, the experimental results agreed qualitatively with the resistivity data obtained from theoretical calculations.

MM 7.2 Mon 12:00 IFW A

Influence of high current densities on nanocrystalline FeC thin films — •Thomas Brede, Reiner Kirchheim, and Cynthia Volkert — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The goal of our study is to understand the influence of high direct current densities on nanocrystalline materials with solute atoms. The latter will be moved by electromigration and causes changes in the microstructure of the host lattice which were in this way the first time described this year [1]. The FeC thin film model system allows to reach current densities up to several MA/cm^2. Different SEM and X-ray techniques are used to observe the changes in microstructure and texture due to the treatment. We will provide detailed experimental results for is model system as well as a mechanism which might explain the observations.
[1] Brede, T., Kirchheim, R., Volkert, C. A. (2020). Anisotropic grain growth in iron-carbon films at high electric current densities. Scripta Materialia, 178, 18-23.

MM 7.3 Mon 12:15 IFW A

Anharmonic self-diffusion coefficients using the finite temperature string method — •Raynol Dsouza[1], Liam Huber[1], Blazej Grabowski[1,2], and Jörg Neugebauer[1] — [1]Max Planck Institut für Eisenforschung, Düsseldorf — [2]Department of Materials Design, Institute of Materials Science, University of Stuttgart

Simulating self-diffusion in solids using molecular dynamics (MD) usually requires high temperatures, where diffusion can occur at a high enough rate. Finite temperature effects can be well represented at low temperatures using phonon calculations in the well-known quasiharmonic approximation (QHA). However, anharmonic effects that appear well below room temperature, even for a relatively simple thermodynamic property like vacancy formation, are not captured by QHA [1].

In this work, we apply the finite temperature string (FTS) method [2] in combination with thermodynamic integration [3] to obtain self-diffusion coefficients that capture anharmonic behavior. Using this technique, diffusion at temperatures above the threshold at which QHA begins to lose validity, as well as temperatures at which calculations by direct MD are feasible can be accessed. Performing a careful analysis, we obtain a good agreement between our results and those simulated by MD at high temperatures, which further extend down to low temperatures for FCC and BCC crystal systems.

[1] Glensk et al. Phys Rev X 4 (2014)
[2] Vanden-Eijnden and Venturoli, J Chem Phys 130 (2009)
[3] de Koning et al. Phys Rev B 70 (2004)

MM 7.4 Mon 12:30 IFW A

Atomistic spin-dynamics simulation of self-diffusion in bcc Fe — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — ICAMS, Ruhr-University, Bochum, Germany

We investigate vacancy diffusion and atomic self-diffusion in bcc iron using a combined lattice-dynamics and spin-dynamics simulation. The spin subsystem is simulated by a classical Heisenberg model that takes into account the exchange interaction between pairs of magnetic spins. The interactions between atoms were described by a new interatomic potential developed in this work using the force-matching method. This method enables to reproduce with high fidelity energies, forces and stresses computed at the ab initio level for a fine-tuned set of reference structures. An extended validation of elastic, thermophysical and defect properties has demonstrated a wide range of applicability of the potential. The diffusion simulations reveal a strong dependence of vacancy formation energy on temperature that leads to a non-Arrhenius behaviour of the self-diffusion coefficient. The simulation results are compared with available experimental data.

MM 7.5 Mon 12:45 IFW A

Autonomous Calculation Of Defect Transport Tensors — •Thomas Swinburne[1] and Danny Perez[2] — [1]CNRS, CINaM, Marseille, France — [2]T-1, Los Alamos National Laboratory, USA

Defect diffusion tensors are essential ingredients for mesoscale material models, but current calculation methods typically have unquantified uncertainty and require significant end user involvement. We combine a massively parallel sampling scheme controlled by Bayesian uncertainty quantification[1] with graph isomorphisms to compress the configuration space of isolated defects and automatically assign off-lattice defect displacement vectors to any found transition. We sample in a space irreducible under space group symmetries and derive an exact expression for the diffusion tensor involving only transitions between states irreducible under translation. A quantitative convergence metric is provided using bounds on the relative entropy.

[1] TD Swinburne and D Perez, Self-optimized construction of transition rate matrices from accelerated atomistic simulations with Bayesian uncertainty quantification. Phys. Rev. Materials 2018, 2, 053802

MM 8: Microstructure and Phase Transformations - Processing

Time: Monday 11:45–13:00 Location: IFW B

MM 8.1 Mon 11:45 IFW B

Crystalline-amorphous interfaces in high entropy alloy nanolaminates produced via high-pressure torsion — •Shabnam Taheriniya[1], Farnaz A. Davani[1], Sven Hilke[1], Harald Rösner[1], Marilena Tomut[2], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Westfälische Wilhelms-Universität Münster, Münster, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany

The intermixing possibilities of dissimilar high entropy alloys and the effect of co-deformation on microstructure evolution were investigated. High pressure torsion (HPT) was applied for bonding separate disks of equiatomic FCC single-phase CoCrFeMnNi and BCC HfNbTaTiZr alloys. The samples were processed for 5, 10 and 15 revolutions at ambient temperature under 9 GPa pressure. The resulting composite material showed enhanced mechanical properties as compared to either HEA systems processed under similar conditions. Scanning electron microscopy and energy-dispersive spectroscopy (EDS) revealed heterogeneous microstructures with relatively sharp chemical interfaces. After large strain, the BCC HfNbTaTiZr phase exhibited significant phase separation into Ta-rich and Ta-poor regions. Moreover, the processed samples possessed a nanolamellar microstructure and vortex-like regions. A partial amorphisation of the BCC phase was observed by transmission electron microscopy.

MM 8.2 Mon 12:00 IFW B

Dissolution of copper additions in aluminium by Friction Stir Processing — •Maximilian Gnedel[1], Amanda Zens[2], Ferdinand Haider[1], and Michael Friedrich Zäh[2] — [1]Chair for Experimental Physics I, Universitätsstraße 1, 86159 Augsburg, Germany — [2]Institute for Machine Tools and Industrial Management, Technical University of Munich, Boltzmannstraße 15, 85748 Garching, Germany

Friction Stir Processing (FSP) is an established method to modify the properties of materials such as aluminium. Furthermore, the composition of the alloy can be changed by this technique. Intermixing specific micrometer-sized metal powders as well as metal foils helps to optimize both the microstructural stability during subsequent heat treatment, as well as the mechanical properties in general. Dispersing copper with different morphologies inside a matrix of AA1050 aluminium by FSP can produce a homogenous solid solution of the two elements, if suitable processing parameters are used. A substantial hardening effect is shown, due to factors such as refinement of the grain structure, solid solution hardening and formation of early stage Al-Cu precipitates. By comparing the particle size distributions before and after FSP and including insights provided by transmission electron microscopy of the Al-Cu interface, a coherent understanding of the alloying process, a complex interplay between diffusion driven dissolution and mechanical fragmentation, can be obtained. The results can be used in future studies to evaluate the properties of such non-equilibrium alloys combined with the unique microstructure produced by FSP.

MM 8.3 Mon 12:15 IFW B

Epitaxial NiTi thin films: a 3D puzzle — •Klara Lünser[1,2], Stefan Schwabe[1,2], Moritz Döllgast[1,2], Kornelius Nielsch[1,2], and Sebastian Fähler[1] — [1]Leibniz IFW Dresden, Germany — [2]TU Dresden, Institute of Materials Science, Dresden, Germany

NiTi is the most widely used shape memory alloy. Its superelastic and shape memory properties are the result of a martensitic transformation from a cubic (B2) to a monoclinic (B19') structure. This transformation gives rise to a complex martensitic microstructure. To customize the material for a specific purpose, a thorough understanding of this microstructure is helpful. In polycrystalline materials, however, the microstructure is influenced by grain boundaries, which complicates an analysis substantially.

Here, we use epitaxial NiTi films as a model system to examine the martensitic transformation and microstructure. These single-crystalline films are grown with DC magnetron sputter deposition in different thicknesses and are probed with scanning electron and atomic force microscopy. Due to the well-defined orientation relation between substrate and film, we can identify the orientations of habit planes and Type I and Type II twin boundaries in the B19' martensite. With in-situ measurements, we additionally examine the nucleation and growth processes of the B19' martensite. Our results are the starting point to understand the three dimensional shape of martensitic nuclei in NiTi B19* martensite which results in a hierarchically twinned microstructure on different length scales.

Supported by DFG (FA 453/13).

MM 8.4 Mon 12:30 IFW B

Microstructural evolution of Mn_3Ga due to annealing in magnetic field — •Gloria Kirste, Christian G.F. Blum, Jens Freudenberger, Sabine Wurmehl, and Bernd Büchner — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

Due to its $D0_{22}$ structure Mn_3Ga can be described as a tetragonally distorted binary Heusler compound. The magnetic properties resulting from this crystallographic structure make the material an interesting candidate for application in spin torque devices or as a rare-earth-free permanent magnet. However, the Mn-Ga phase diagram is rather complex such that the $D0_{22}$ phase cannot be obtained by melting but needs further heat treatment. Moreover, the magnetic characteristics are affected by the material's microstructure and texture.

Within this study arc melted Mn_3Ga was deformed by rotary swaging to promote the phase transformation. After annealing for up to two weeks the change in microstructure was analysed. The results of X-ray diffraction provide information on the present crystallographic phases whereas microscopical methods revealed the grain size distribution. Some of the resulting magnetic characteristics were examined using SQUID magnetometry.

Several samples experienced annealing in a high static magnetic field as another aid to phase transformation and also in order to achieve a more pronounced texture. The value of magnetic field annealing as a tool for stimulating phase transformation and tuning microstructure will be discussed.

MM 8.5 Mon 12:45 IFW B

Phase selection and microstructural evolution of CoCrNi medium entropy alloy under cointernerless processing — •Angelo Fernandes Andreoli[1], Olga Shuleshova[1], Yuhao Wu[1,2], and Ivan Kaban[1] — [1]IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Department of Applied Physics, Northwestern Polytechnical University, Xi'an, 710072, China

The CoCrNi alloy was cointainerlessly processed using a portable electromagnetic levitation device where in-situ X-ray diffraction and a high-speed camera were used to monitor the phase evolution and solidification behavior. At low undercoolings, the alloy nucleates the stable γ-fcc phase, which consequently grows until the solidification is over. Beyond a critical undercooling, it first nucleates the metastable δ-bcc phase, which completely transforms into the stable γ-fcc phase as solidification evolves. Crystal growth kinetics were determined and are comparable to Fe-Co binary alloys. The microstructural evolution exhibits a transition from a dendritic microstructure at low undercoolings to an equiaxed-refined structure at deeper undercoolings.

MM 9: Liquid and Amorphous Metals - Brittle-to-ductile Transition

Time: Monday 11:45–13:00 Location: IFW D

MM 9.1 Mon 11:45 IFW D

Invar effect in Fe-based bulk metallic glasses — •Alexander Firlus, Robin Schäublin, Mihai Stoica, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Ferromagnetic Fe-based bulk metallic glasses universally show a low coefficient of thermal expansion, which suddenly increases by a factor of ∼3 at the Curie temperature. This effect is known as Invar effect and it is usually seen in crystalline FeNi alloys. While it is clear that this is a magnetically driven effect, the physics behind it is still not understood. Up to now, the only explanations of the Invar effect are based on simulations and calculations that rely on a unit cell, but these have no base in amorphous materials. The strength of the Invar effect is particularly sensitive to the short-range order and Fe coordination. We thus aim to investigate the dynamics from the atomic scale to the macroscale for various alloys in different structural states. We correlate the structural data determined via transmission electron microscopy with studies on the magnetics to get a complete picture of the underlying mechanics of the Invar effect in Fe-based magnetic glasses.

MM 9.2 Mon 12:00 IFW D

How does a Cu-Zr-Al glass/crystal composite form in real time? — •Jiri Orava[1], Ivan Kaban[1], Xiaoliang Han[1], Olga Shuleshova[1], Ivan Soldatov[2], Olof Gutowski[3], Ann-Christin Dippel[3], Martin v. Zimmermann[3], Shanoob Balachandran[4], Michael Herbig[4], Yurii Ivanov[5], Alan L. Greer[5], and Dierk Raabe[4] — [1]IFW Dresden, Germany — [2]IFW Dresden, Germany — [3]DESY, Hamburg, Germany — [4]MPIE, Düsseldorf, Germany — [5]Department of Materials Science and Metallurgy, University of Cambridge, UK

Metallic glasses (MGs) have poor ductility, and due to the lack of atomic periodicity and microstructure, MGs mechanical properties cannot be controlled the same way as in crystalline materials. One approach to enhance ductility of MGs lies in introducing ductile nanometre-to-micrometre-size crystalline phases into a glass. This method has proven to be an effective way to improve the mechanical properties of such composites, particularly their plastic formability. We present a real time in-situ high-energy x-ray diffraction study of phases evolution during a controlled rapid-heating treatment, imposed at a rate ranging from ~100-1000 K/s, and subsequent cooling of a Cu-Zr-Al metallic glass. We combine the synchrotron measurements with in-situ heating in TEM and with atom-probe tomography analysis of the final composite microstructures. The formation of crystalline phases beneficial to the ductility are clearly resolved and conditions under which these phases develop are formulated. We thank the DFG, contracts Ka-3209/9-1 and HE 7225/1-1, for funding.

MM 9.3 Mon 12:15 IFW D

Boron concentration induced Co-Ta-B composite formation observed in the transition from metallic to covalent glasses — •Simon Evertz[1], Stephan Prünte[1], Lena Patterer[1], Marshal Amalraj[1], Damian M. Holzapfel[1], Alexander Schökel[2], Marcus Hans[1], Daniel Primetzhofer[3], and Jochen M. Schneider[1] — [1]Materials Chemistry, RWTH Aachen University, Aachen, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Due to their unique property combination of high strength and toughness, metallic glasses are promising materials for structural applications. As the behaviour of metallic glasses depends on the electronic structure which in turn is defined by chemical composition, we investigate systematically the influence of B content on glass transition, topology, magnetism and bonding for B contents between 2 and 92 at% in the $(Co_{6.8}Ta_1)_{1-x}B_x$ system. From an electronic structure and coordination point of view the B concentration range is divided into three regions: Below $38 \pm 5at\%$ B, the material is a metallic glass due to the dominance of metallic bonds. Above $67 \pm 5at\%$ the presence of an icosahdra-like B-network is observed. As the B concentration is increased above $38 \pm 5at\%$, the B-network evolves while the metallic coordination of the material decreases until the B concentration of $67 \pm 5at\%$ is reached. Hence, a composite is formed. It is evident that based on the B concentration the ratio of metallic bonding to icosahedral bonding in the composite can be controlled.

MM 9.4 Mon 12:30 IFW D

Cooling rate, temperature and applied strain rate effects on the brittle-to-ductile transition in metallic glasses — •Xudong Yuan[1], Daniel Şopu[1,3], and Jürgen Eckert[1,2] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Montanuniversität Leoben, Leoben, Austria — [3]Technische Universität Darmstadt, Darmstadt, Germany

The effects of cooling rate, temperature and applied strain rate on the tensile deformation behavior of Cu64Zr36 metallic glass (MG) are investigated using large-scale molecular dynamics simulations. An increase in quenching rate during sample preparation, as well as an increase of temperature or applied strain rate, affects the shear band nucleation and propagation processes and causes a brittle-to-ductile transition. High quenching rates lead to a low density of closed packed Cu-centered full icosahedra and by sampling of the saddle points on the potential energy surface we found lower barrier energy for local atomic rearrangement as compared to those MGs obtained at low quenching rates. High temperatures will increase the kinetic energy of the atoms, which leaves the atoms to easily rearrange and increases the probability of thermal activation of shear transformation zones. Finally, during deformation at high strain rates, the stored elastic energy has not enough time to redistribute through local elastic distortions along the maximum shear stress direction and, consequentially, the MGs deform homogeneously.

MM 9.5 Mon 12:45 IFW D

Temperature and chemical bonding effects on the brittle-to-ductile transition in metal-metalloid glasses — Franco Moitzi[1], •Daniel Şopu[1,2], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Montanuniversität Leoben,

Leoben, Austria

The relationship between the deformation behavior of metal-metalloid glasses and their intrinsic properties is studied using large-scale molecular dynamics simulations with hybrid interatomic potentials. Particularly, the influence of composition and temperature on the tensile deformation behavior of amorphous PdSi alloys is investigated. A transition from cracking perpendicular to the loading direction to shear banding can be achieved by increasing the temperature or decreasing the amount of silicon. A decrease in silicon content leads to fewer covalent bonds and, therefore, lower activation barriers for shear transformation zones and, consecutively, a high probability for shear band formation. On the other hand, at low temperatures these barrier cannot be overcome and cracking will dominate over shear banding. In this case, high activation barriers for local relaxation impedes stress redistribution into the glassy structure and, finally, cracking occurs. Additionally, the cracking path also depends on the degree of homogeneity. A corrugated fracture surface similar to experiment can be formed due to crack defection and cavitation ahead of the crack tip in chemically inhomogeneous samples. In contrast, a sharp cleavage-like fracture occurs for more homogeneous samples.

MM 10: Invited talk Körmann

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

Invited Talk MM 10.1 Mon 15:00 BAR 205

High-Entropy Alloys: Materials design in high dimensional chemical space from ab initio thermodynamics — •Fritz Körmann — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — Materials Science and Engineering, Delft University of Technology, 2628 CD, Delft, The Netherlands

A well-targeted design of modern alloys such as high entropy alloys (HEAs) is extremely challenging due to their immense composition space. In this talk I will discuss recent advances in fully parameter-free ab initio calculations combining advanced statistical concepts and machine learning techniques. These novel techniques allow to computationally identify favorable composition islands in the high dimension chemical phase space solely on the computer. Using this approach, various mechanisms and concepts proposed in the literature have been tested: Besides lattice distortions, stacking-fault energies (SFEs) have been successfully used as a descriptor to link atomistic simulations to the macroscopic deformation mechanisms that are behind the superior mechanical performance. Interstitial alloying with C reveals, e.g., large fluctuations in solution energies depending on the specific local chemical environment and its impact on SFEs can be even qualitatively different depending on alloy composition. We also discuss BCC-HCP stability as promising descriptor to identify mechanically appealing refractory HEAs and the critical role of lattice distortions therefore. Based on these computationally highly expensive computations easy-to-use materials design rules will be derived and discussed for the various examples.

MM 11: Topical Session: Data Driven Materials Science - Machine Learning for Damage Prediction

Time: Monday 15:45–16:45 Location: BAR 205

Topical Talk MM 11.1 Mon 15:45 BAR 205

From microscopic models of damage accumulation in Ni-base superalloys to the failure probability of gas turbine components — •Tilmann Beck[1], Benedikt Engel[2], Nadine Moch[3], Lucas Mäde[4], Sebastian Schmitz[4], and Hanno Gottschalk[3] — [1]TU Kaiserslautern, Kaiserslautern, Germany — [2]University of Nottingham, Nottingham, UK — [3]Bergische Universität Wuppertal, Wuppertal, Germany — [4]Siemens AG Gas & Power, Berlin, Germany

Conventionally cast (CC) Ni-base superalloys subjected to cyclic mechanical loading exhibit considerable scatter in fatigue lifetime. This is caused by i) a very coarse crystal structure ii) an extremely pronounced elastic anisotropy with Young's moduli (T = 850°C) of approx. E = 100 GPa in [001] and up to 250 GPa in [111] lattice direction and (iii) the fact that fatigue cracks are predominantly initiated in type {111} <110> slip systems of the fcc lattice.

A modeling approach is presented considering anisotropy of E and the Schmid factor m of the {111} <110> slip systems. Based on this, and EBSD analyzes of the actual grain orientation distribution, it is possible to (i) identify crystal grains prone to fatigue cracking and (ii) to explain the major part of the scatter in fatigue lifetime. Using Monte-Carlo simulations of grain orientations, frequency distributions of E and m were determined and collapsed into a damage parameter which quantifies the grain orientation dependent scatter in fatigue life. Using probabilistic approaches based on Weibull's weakest link concept, a model was developed for prediction of the influence of component size and inhomogeneous load distributions on the fatigue lifetime.

MM 11.2 Mon 16:15 BAR 205

Large-area, high-resolution characterisation and classification of damage mechanisms in dual-phase steel using deep learning — •Setareh Medghalchi[1], Carl F. Kusche[1], Tom Reclik[1], Martina Freund[1], Ulrich Kerzel[2], Talal Al-Samman[1], and Sandra Korte-Kerzel[1] — [1]Institut für Metallkunde und Metallphysik, RWTH, Aachen,Germany — [2]IUBH University of Applied Sciences,Bad Honnef,Germany

Dual-phase steels are popular in the automotive industry as they allow lightweight design with high stiffness and good ductility. However, their damage behavior is not yet fully understood and their heterogeneity at different length scales impedes a full characterization based on small excerpts of the microstructure. Understanding their damage behavior therefore requires detailed investigations of many damage sites at high-resolution over large areas. To this end, we have collected a large amount of data by means of panoramic imaging in a scanning-electron-microscope before and after deformation following different strain paths. Machine-learning allows us to tackle the challenges of automated analysis of the microstructure of dual phase steel samples. A deep-learning based algorithm has been developed to classify the detected damage sites in the microstructure. Furthermore, we have now enhanced the accuracy and robustness of our method by data-augmentation, making it applicable on samples which were subjected to different deformation conditions, e.g. uniaxial or biaxial tensile testing. This reduces the need for manual interventions, aiding the high-statistics-microstructural-analysis under variable conditions.

MM 11.3 Mon 16:30 BAR 205

Statistical characterisation of damage sites in dual phase steels under different mechanical deformations — •Setareh Medghalchi[1], Carl F. Kusche[1], Tom Reclik[1], Martina Freund[1], Ulrich Kerzel[2], Talal Al-Samman[1] und Sandra Korte-Kerzel[1] — [1]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany — [2]IUBH University of Applied Sciences, Bad Honnef, Germany

During last years the increasing demand for high strength and good ductility beside light weight, introduces dual phase steels as a proper candidate for automotive industries. Understanding the failure behavior of these parts requires detailed investigations about the damage sites of its microstructure in high resolutions over the large deformed areas. In our framework, large amount of data are collected by means of automatic panaromic imaging in scanning electron microscope. Taking the advantage of artificial intelligence facilitates us to tackle the challenges of data collection and interpretation of the microstructure of the dual phase steel. A deep-learning based algorithm has been developed to classify the detected damage sites in the microstructure. Furthermore, we have enhanced the flexibility and accuracy of our method to make it applicable on samples which underwent different mechanical deformations like biaxial tensile test. The extended version of this method is invariant with respect to different features of the damage sites (like geometry, orientation, color contrast) which provides statistically relevant mechanisms of damaging that leads to microstructural analysis in addition to the laborious efforts reduction.

MM 12: Transport - High Entropy Alloys

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

MM 12.1 Mon 15:45 IFW A

Solute and self-diffusion in HCP high entropy alloys — •Sandipan Sen[1], Mayur Vaidya[1], Lukasz Rogal[2], Xi Zhang[3], Blazej Grabowski[3,4], Sankaran Shanmugam[5], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, 30-059 Krakow, Poland — [3]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [4]Institute of Materials Science, University of Stuttgart, 70569 Stuttgart Germany — [5]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai-600036, India

Diffusion studies in high entropy alloys (HEAs) are still scarce and practically limited to FCC systems. For the first time, diffusion in HCP HEAs is investigated using a radiotracer technique. Solute diffusion of Co and self-diffusion of Zr are systematically measured in binary HfZr, ternary HfZrTi, and quinary Al-Hf-Sc-Ti-Zr alloys in the temperature range of 400*C to 1100 *C. The phase composition of the alloys is characterized by X-ray diffraction and transmission electron microscopy. Two quinary systems (Al15Hf25Sc10Ti25Zr25 and Al5Hf25Sc20Ti25Zr25) are studied to examine the influence of the Al addition and potential ordering. A comparative study of the solute and self-diffusion is made to understand the impact of chemical disorder and of potential ordering on the diffusion properties in these systems.

MM 12.2 Mon 16:00 IFW A

tracer diffusion in the σ-phase of the CoCrFeMnNi system — jingfeng zhang[1], mohan muralikrishna garlapati[1,2], alex asabre[3], guillaume laplanche[3], sergiy divinski[1], and •gerhard wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Metallurgical & Materials Engineering, Indian Institute of Technology Madras, Chennai, India — [3]Institut für Werkstoffe, Ruhr-Universität Bochum, Bochum, Germany

Formation of a Cr-rich σ-phase in the CoCrFeMnNi high-entropy alloy during long term exposures at intermediate temperatures (< 1073 K) is detrimental for the mechanical properties. The σ-phase represents a topologically close-packed complex phase with a tetragonal structure. The diffusion processes which take place in the σ-phase are very important to understand the kinetics of precipitation of this phase in the cantor alloy. So far, there are no reports on diffusion in the σ-phase composed of elements in Cantor alloys.

In the present work, the σ-phase with the composition Co46Cr15.2Fe16.3Mn17Ni5.5 (in at.%) was produced and investigated. For the first time, tracer diffusion of Ni and Fe was measured in the temperature interval from 928 - 1173 K using 64Ni and 58Fe natural isotopes in combination with depth profiling by a secondary ion mass spectroscopy. Diffusion of both Ni and Fe in the σ-phase is found to be faster compared to that in the Cantor alloy. Various reasons influencing diffusion in the σ-phase and its effect on phase stability of the Cantor alloy system are discussed.

MM 12.3 Mon 16:15 IFW A

Radiotracer diffusion in single crystalline CoCrFeNi and CoCrFeMnNihigh entropy alloys — •Daniel Gaertner[1], Josua Kottke[1], Yury Chumlyakov[2], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster,Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, Tomsk, Russia.

High entropy alloys are multicomponent alloys, which consist of five or more elements in equiatomic or nearly equiatomic concentrations. These materials are hypothesized to show significantly decreased self-diffusivities. For the first time, the temperature dependencies of the volume diffusion rates of all constituent elements in equiatomic CoCrFeNi and CoCrFeMnNi single crystals and additionally solute diffusion of Mn an Cu in the quaternary alloy and Zn in the quinary alloy are investigated using the radiotracer technique in an extended temperature range between 923 K and 1373 K. The components are characterized by significantly different diffusion rates with the activation enthalpies in a range between 200 and 300 kJ/mol. Cu is found to be a fast diffuser at moderate temperatures below 1273 K and its diffusion rate follows the Arrhenius law with an activation enthalpy of 149 kJ/mol. Furthermore, a distinct contribution of short-circuit pipe diffusion was observed and analyzed.

MM 12.4 Mon 16:30 IFW A

Tracer diffusion in the Ni–CoCrFeMn system: transition from a dilute solid solution to a high entropy alloy — •Josua Kottke[1], Adnan Fareed[1], Shabnam Taheriniya[1], Ziyuan Rao[2], Zhiming Li[2], Mathilde Laurent-Brocq[3], Loïc Perrière[3], Łukasz Rogal[4], Harald Rösner[1], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [3]Université Paris Est, ICMPE (UMR 7182), CNRS, UPEC, F-94320, Thiais, France — [4]Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, 30-059 Krakow, Poland

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 physical and mechanical properties, especially at elevated temperatures. Here, we report on the kinetic properties and the microstructural response regarding the transition from a pure metal (Ni) to a dilute solid solution and finally to a high entropy alloy within a single-phase FCC domain. Tracer diffusion rates of all elements are measured in $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$, $Co_{10}Cr_{10}Fe_{10}Mn_{10}Ni_{60}$ and $Co_2Cr_2Fe_2Mn_2Ni_{92}$ alloys and are compared to those in pure Ni. The volume diffusion data substantiate that the proposed 'sluggish' diffusion is at least an ambiguous concept. Grain boundary diffusion shows a number of unexpected features which are related to the microstructure characteristics and have been further analyzed by TEM and APT.

MM 13: Microstructure and Phase Transformations - Processing and Imaging

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

MM 13.1 Mon 15:45 IFW B

High-gravity processing of metals at elevated temperatures — •Štefan Stanko, Mihai Stoica, Josef Hecht, Erwin Fischer, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Research into ultracentrifugation is generally limited to molecular biology, biochemistry and polymer science. To investigate the behavior of metals at ultrahigh gravity, a unique centrifuge was designed and built in-house. The apparatus is capable of achieving an acceleration of more than 50,000 g together with a temperature of up to 1,200 °C. At this acceleration, the sedimentation of atoms in solid solution is expected to play an important role, and the pressure gradient within the sample has an effect on the thermodynamics of the system. Under ultrahigh gravity, more phases may be observed than predicted by the Gibbs phase rule due to the effect that the chemical potentials of the various phases become gravity dependent. The processing method can also be used to explore eutectic compositions in complex multicomponent alloys. In this work, we investigate the effect of acceleration on the crystallization of pure metals such as aluminum and tin. The metals were molten and slowly cooled to room temperature at an acceleration of 26,000 *g*. They were then characterized via metallurgical methods as well as scanning and transmission electron microscopy. The results on the sedimentation and nanoscale microstructure obtained via this high-temperature centrifugal processing are presented and discussed.

MM 13.2 Mon 16:00 IFW B

Silicon Highly Enriched in 28Si: Probing Artificial Crystals for the Dissemination of the Mole and Kilogram — •Axel Pramann and Olaf Rienitz — Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

The revision of the SI units mole and kilogram has been enabled by the exact realization of the Avogadro constant by the the X-ray-crystal-density (XRCD) method *counting* silicon atoms in single-crystalline silicon spheres [1] and the complementary realization of the Planck constant using a Kibble balance [2]. For the XRCD method applied by PTB, a pool of few unique silicon single crystals highly enriched in 28Si has been produced and characterized. Using a high-resolution MC-ICP mass spectrometer and a tailored analytical methodology in a key experiment, the isotopic composition (the molar mass M) of these crystals has been determined with associated uncertainties of u(M) < 1 x 10-9, which is unique in chemistry up to now. After developing and improving this method during the last decade, the uncertainties u(M) were reduced by almost three orders of magnitude. The way how to disseminate the amount of substance and kilogram after the revision of the SI is outlined [1, 3]. [1] K. Fujii et al., Metrologia, 53, A19 (2016). [2] I. A. Robinson, S. Schlamminger, Metrologia, 53, A46 (2016). [3] B. Güttler, O. Rienitz, A. Pramann, Annalen der Physik, 1800292 (2018)

MM 13.3 Mon 16:15 IFW B

Random walks on images - statistical analysis and Hurst component calculation — •Tomasz Blachowicz[1], Fjora Mance[2], David Fetter[3], Alexander Friesen[3], Axel Dreyer[4], Artur Kasza[1], and Andrea Ehrmann[3] — [1]Silesian University of Technology, Institute of Physics - Center for Science and Education, 44-100 Gliwice, Poland — [2]Polytechnic University of Tirana, Faculty of Mechanical Engineering, Tirana, Albania — [3]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany — [4]Bielefeld University, Department of Physics, 33615 Bielefeld, Germany

Pictures of diverse structures can be investigated by image processing, followed by mathematical methods, to derive geometrical or other properties of these objects. Especially irregular samples, such as fibrous materials [1], can be examined by a random-walk algorithm, enabling calculation of the so-called Hurst exponent [2].

Here we show the analysis of drying processes of different polymer pre-cursors on varying surface by grey-channel dependent Hurst exponent calculations, performed on microscopic images of the drying traces. Our results allow for quantifying the differences between drying marks of diverse fluids and thus classifying various crystallization processes.

[1] T. Blachowicz, A. Ehrmann, K. Domino, Physica A: Statistical Mechanics and its Applications 452, 167-177 (2016)

[2] A. Ehrmann, T. Blachowicz, K. Domino, S. Aumann, M. O. Weber, H. Zghidi, Textile Research Journal 85, 2147-2154 (2015)

MM 13.4 Mon 16:30 IFW B

Hidden charge order in an iron oxide square-lattice compound — •Darren C. Peets[1,2,3], Jung-Hwa Kim[1], Manfred Reehuis[4], Peter Adler[5], Andrey Maljuk[1,6], Tobias Ritschel[3], Morgan C. Allison[3], Jochen Geck[3], Jose R. L. Mardegan[7], Pablo J. Bereciartua Perez[7], Sonia Francoual[7], Andrew C. Walters[1], Thomas Keller[1,8], Paula M. Abdala[9], Philip Pattison[9,10], Pinder Dosanjh[11], and Bernhard Keimer[1] — [1]MPI-FKF, 70569 Stuttgart — [2]NIMTE, CAS, Ningbo, 315201 China — [3]IFMP, TU Dresden, 01069 Dresden — [4]HZB, 14109 Berlin — [5]MPI-CPfS, 01187 Dresden — [6]IFW, 01171 Dresden — [7]DESY, 22603 Hamburg — [8]MLZ, 85748 Garching — [9]ESRF, 38042 Grenoble, France — [10]EPFL, 1015 Lausanne, Switzerland — [11]UBC, Vancouver, V6T 1Z1 Canada

We report Fe^{3+}–Fe^{5+} charge order in square-lattice $Sr_3Fe_2O_7$. The charge order is nearly invisible to state-of-the-art diffraction probes, despite its simple checkerboard structure, large amplitude, and high critical temperature $T_{CO} \sim 330\,K$. This arises from the highly-symmetric lattice structure of $Sr_3Fe_2O_7$, combined with frustration of interlayer Coulomb interactions. We point out parallels to electronic nematicity and hidden order in *d*- and *f*-electron compounds with frustrated interactions.

MM 14: Computational Materials Modelling - Methods I

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

MM 14.1 Mon 15:45 IFW D

Accuracy vs. efficiency? Towards ACKS2-based polarization in force fields — •Patrick Gütlein[1], Karsten Reuter[1], Harald Oberhofer[1], and Jochen Blumberger[2] — [1]Technische Universität München, Germany — [2]University College London, UK

Electronic polarization poses a minor energy contribution compared to the formation and arrangement of covalent bonds, yet it crucially influences both geometric and electronic properties of soft condensed matter and molecular crystals. Frequently, effective force field techniques employed to sample the phase space of such systems insufficiently cover the complex dielectric response to external perturbations. Here, the recently proposed atom-condensed Kohn-Sham density functional theory approximated to second order (ACKS2) approach promises to be a computationally undemanding, still accurate electronic polarization extension to conventional force field methods. It rests on an atom-centered basis set expansion of the linear responses of both the electron density and the Kohn-Sham potential.

In order to provide a generally applicable ACKS2 extension to force fields, we develop a new and efficient Gaussian type basis set representation. We demonstrate the efficacy of ACKS2 with the new basis set for a range of molecular model systems, which are relevant building blocks in common organic semiconductors and biotic materials. Furthermore, we formulate a fragmentation scheme to improve both computational scaling with system size and evaluation of the condensed response parameters. This marks important first steps to employ ACKS2 as polarization correction in force fields.

MM 14.2 Mon 16:00 IFW D

Modified Becke-Johnson calculations using pseudopotential plane-wave approach: Systematic analysis — •Hazem Abu-Farsakh[1], Mohammad Abu-Jafar[2], and Abdallah Qteish[3] — [1]Dept. of General Sciences, Prince Sultan University, Riyadh, Saudi Arabia — [2]Dept. of Physics, An-Najah National University, Nablus, Palestine — [3]Dept. of Physics, Yarmouk University, Irbid, Jordan

The modified Becke-Johnson exchange potential (mBJ) has been promising for providing accurate band gaps for various types of solids at low cost. The optimization of the mBJ potential was done using the all-electron (AE) electronic structure technique and it is usually tested within the AE method (mBJ@AE). On the other hand, the performance of the mBJ with the pseudoptential approach (mBJ@PP) is not well explored. We therefore present systematic investigation of the electronic structure of different semiconductors and insulators employing the mBJ@PP approach. mBJ@AE and screened hybrid functional YS-PBE0 calculations are also performed for comparison. It is found that using typical PP's the mBJ@PP calculations lead to bandgaps that are significantly smaller than in the mBJ@AE approach. The best agreement with the mBJ@AE band gaps is obtained by including the outer core *p* electrons as valence in the cation PPs. For the considered systems, apart from Cu_2O and ScF_3, the obtained bandgaps are in very good agreement with those of YS-PBE0, G_0W_0, and experiment. We also investigate the calculated binding energies of the semicore *d* electrons, upper valence bandwidths, and electron effective masses. Explanations of the mBJL@PP results are provided.

MM 14.3 Mon 16:15 IFW D

Optimized effective potentials to increase the accuracy of ap-

proximate proton transfer energy calculations in the excited state — •Pouya Partovi-Azar and Daniel Sebastiani — Institute for Chemistry, MLU Halle-Wittenberg

In various systems, acidic properties emerge when the system is electronically excited. Although the time scale attributed to the dynamics of the electrons is usually on the order of femtoseconds, the electronic excitations can in general trigger much slower processes.

Here, we propose and benchmark a novel approximate first-principles molecular dynamics simulation idea for increasing the computational efficiency of density functional theory-based calculations of the excite states. We focus on obtaining proton transfer energy at the S_1 excited state through actual density functional theory calculations at the T_1 state with additional optimized effective potentials. The potentials are optimized such as to reproduce the time-dependent density functional theory energy surface, but can be generalized to other more accurate quantum chemical methods. We demonstrate the applicability of this method for two prototypical photoacids, namely phenol and 7-hydroxyquinoline. We show that after optimizing the additional effective potentials for carbon, nitrogen, oxygen, and the acidic hydrogens, both thermodynamics and kinetics of proton dissociation reaction can be well reproduced as compared to reference excited-state calculations. It is found that a good agreement can be reached by only optimizing two effective potential parameters per each species in the photoacids.

MM 14.4 Mon 16:30 IFW D

Assessing the accuracy of screened range-separated hybrids for bulk properties of semiconductors — •Stefan Alois Seidl, Bernhard Kretz, and David Alexander Egger — Department of Physics, Technical University of Munich, 85748 Garching, Germany

While conventional semilocal and hybrid functionals in density functional theory (DFT) are known to predict structural properties of semiconductors accurately, they fail to quantitatively describe electronic-structure and optical properties of these materials. Screened range-separated hybrid (SRSH) functionals were recently shown to provide highly accurate electronic-structure and optical properties of prototypical semiconductors [1]. In the SRSH approach, a single empirical parameter is used to fit the SRSH band gap such that it reproduces the GW band gap, by tuning the range-separation parameter while maintaining 25% exact exchange in the short-range [1]. Here, we assess the accuracy of the SRSH approach in computing bulk properties (e.g., lattice constants, bulk moduli, atomization energies etc.) of several prototypical semiconductors. To this end, results from the SRSH method are compared to experimental data as well as to computational results obtained when using conventional semilocal and hybrid DFT functionals.

[1] D. Wing et al, Phys. Rev. Materials 3, 064603 (2019)

MM 15: Topical Session: Data Driven Materials Science - Machine Learning for Production (joint session MM/CPP)

Time: Monday 17:00–17:30 Location: BAR 205

Topical Talk MM 15.1 Mon 17:00 BAR 205

First-principle infused machine learning models allowing digital twins to self-organise production processes — •Marcus Neuer — Sohnstr. 65, 40237 Düsseldorf

For European process industries, optimization of the production route plays an increasingly important role for keeping a competitive edge in a tough market. New concepts like digital twins arrived recently in real-world applications. They allow an agent-based, active self-organisation of the route and introduced the ability to apply models live, during the processing. These models may be analytically derived, data-based or a combination of both: first-principle infused machine learning models. Herein, the stochasticity of the process is modelled by the machine learning approach, while an analytical first-principle backbone acts as basis. With the ability to forecast its potential future, materials and products have new degrees of freedom. They optimize their future path with respect to energy consumption, order matching and material homogeinety. The presented concepts are shown in real-world production environments, where they have already reached technical readiness to sustain continuous production.

MM 16: Transport - Heat Transport and Thermoelectricity

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

MM 16.1 Mon 17:00 IFW A

Specific heat capacity measurements and transmission electron microscopy investigation of FeMn alloys — •Marius Gerlitz, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Westfälische Wilhelms-Universität, Münster, Deutschland

Magnetocaloric materials are promising for various fields of application and their thermodynamic fundamentals are crucial to understand. In this work, low temperature specific heat capacity measurements are performed for a series of Fe-Mn alloys with and without application of a magnetic field (up to 9T) in the temperature interval from 4 K to 400 K. A physical properties measurement system (PPMS) is used and the 2-tau method is applied for the analysis. Furthermore, the heat capacity measurements are extended to higher temperatures from 300 K to 723 K using differential scanning calorimetry and applying heating rates of 20 K/min. As a result, thermal and magnetic entropy contributions are determined alongside with the determination of further characteristic properties such as the Debye temperature or the electronic contribution to the specific heat. A microstructural analysis is performed by transmission electron microscopy (TEM). The results are discussed with respect to the chemical composition and potential short-range ordering.

MM 16.2 Mon 17:15 IFW A

Thermal conductivity of Th and ThC — •Lukas Kyvala and Dominik Legut — VSB - Technical University of Ostrava, 17. listopadu 15, 70833 Ostrava-Poruba, Czech Republic

Thermal conductivity is one of the most important properties of nuclear fuel materials affecting many processes such as swelling, grain growth, and fission gas release and limits the transfer of the linear power.

Experimental measurement of thermal conductivity is difficult because of the loss of heat through convection, conduction, and radiation. The different measurements do not find full agreement even for such a simple case like silicon. Moreover, the measurement of radioactive elements is complicated due to the self-heating. Theoretical calculations are then a very useful tool.

We demonstrate the success of predicting the thermal conductivity of potential nuclear fuels like Th and ThC using electron-structure calculations. Both phonon (lattice) and electron contributions were calculated as a function of temperature.

Next, we discuss why the total thermal conductivity of thorium metal is more than twice as large as thorium monocarbide and why the optical phonon modes of ThC accounting only for approximately 6 % of the total phonon contribution. This result differs significantly from NpO_2 where the optical branches contribute only 27 %.

MM 16.3 Mon 17:30 IFW A

Temperature and doping dependence of the thermoelectric power of $Yb(Rh_{1-x}Co_x)_2Si_2$ intermetallic compounds — •Veljko Zlatic[1] and Ulrike Stockert[2] — [1]Department of Physics, Faculty of Science, University of Split, Croatia — [2]MPI for Chemical Physics of Solids, Dresden, Germany

The temperature and doping dependence of transport coefficients of $Yb(Rh_{1-x}Co_x)_2Si_2$ series of alloys is explained by an asymmetric Anderson model which takes into account the exchange scattering of conduction electrons on Ytterbium ions and the splitting of $4f$-states by the crystalline electric field (CEF). The substitution of rhodium by cobalt is described as an increase of chemical pressure which reduces the exchange coupling and the CEF splitting. The scaling analysis and numerical NCA solution of the model show that, at a given temperature, the effective degeneracy of the $4f$-state depends on the relative magnitude of the Kondo scale and the CEF splitting. The temperature and doping dependence of the thermopower of $\mathrm{Yb(Rh_{1-x}Co_x)_2Si_2}$ series of alloys is explained as an interplay of quantum fluctuations, driven by the exchange scattering, and thermal fluctuations which populate the excited CEF states. The theoretical results obtained in such a way capture all the qualitative features of the experimental data.

MM 16.4 Mon 17:45 IFW A

Thermoelectricity in high-valley multiplicity materials — Roberta Farris[1], Francesco Ricci[2], Geoffroy Hautier[2], Gian-Marco RIgnanese[2], and •Vincenzo Fiorentini[1] — [1]Dip. di Fisica, Università di Cagliari, Italy — [2]University of Louvain-la-Neuve, Belgium

We present a detailed theoretical study of two promising thermoelectrics, LaSO and YB4Mo, which turn out to have a large multiplicity and band complexity factor from a data mining search on a large electronic-structure database. Bands are computed ab initio and transport is studied in the Bloch-Boltzmann approximation; lattice thermal is modeled from the ab initio harmonic spectrum. The two materials reach a ZT of over 2 at typical temperatures.

MM 17: Computational Materials Modelling - Methods II

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

MM 17.1 Mon 17:00 IFW D

Phase Transitions Investigated by Variationally Enhanced Sampling with Permutationally Invariant Collective Variables — •Bin Song[1], Gareth Tribello[2], Kurt Kremer[1], and Omar Valsson[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Queen's University of Belfast, Belfast, United Kingdom

Phase transitions are a common theme in our physical world, which are performed over various acts in crystallization of atomic or molecular crystals and transformations between various phases of nanoalloys or soft matters. These phenomena could affect catalytic activity of a catalyst, the bioavailability of a drug molecule, and the stability of metal structures. For understanding phase transitions, molecular dynamic (MD) simulations have become an indispensable tool that is versatile and capable to provide mechanistic insights. Despite the advancement of computing hardware and development of algorithms, the timescale of MD simulations is still limited. Our group has been developing Variationally Enhanced Sampling (VES) method to transcend this limit placed upon MD practitioners. VES builds a bespoke bias potential in the collective variable (CV) space to drive the systems to visit different states and achieve ergodicity, with the collective variables being functions of the configuration space. In this work, we have extended the functionality of VES to use local Permutationally Invariant Collective Variables in situations when global CVs are not viable. We demonstrate the merits of method through studies of phase transition of LJ clusters, and crystallization and melting of bulk sodium.

MM 17.2 Mon 17:15 IFW D

New basis functions and optimization algorithms for Variationally Enhanced Sampling — •Benjamin Pampel and Omar Valsson — Max Planck Institute for Polymer Research, Mainz, Germany

Variationally Enhanced Sampling is an advanced sampling method for molecular dynamics simulations based on a variational principle. A bias potential is construed by minimizing a convex functional, to obtain thermodynamic and kinetic information of rare event systems.

So far mostly orthogonal polynomials have been used as basis functions for the expansion of the bias potential. While there have been proposals for alternatives, this was for specific problems and not with a general evaluation of the performance of the method in mind. Therefore, the most efficient choice of basis functions is an open question.

Another important ingredient of the VES method is the employed optimization algorithm. While the Bach's averaged stochastic gradient decent used so far has generally performed fine, more recent algorithms from the field of machine learning might perform better.

To answer these two open questions, we first implemented and evaluated the performance of new sets of basis functions, including Gaussians and cubic splines, by testing them on various systems. We find the usage of Daubechies Wavelets favorable for many applications.

For the optimization, besides implementing some of the popular algorithms like Adagrad or Adam, we also propose our own modifications. Here the conclusions are less clear, as only in few cases the Adam algorithm is able to outperform Bach's algorithm.

MM 17.3 Mon 17:30 IFW D

Self-consistent site-dependent DFT+U(+V) for defects — Chiara Ricca[1], Iurii Timrov[2], Matteo Cococcioni[2,3], Nicola Marzari[2], and •Ulrich Aschauer[1] — [1]University of Bern, Bern, Switzerland — [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]University of Pavia, Pavia, Italy

DFT calculations of defects in transition metal oxides often require advanced methods such as hybrid functionals to yield a reasonable description of the electronic structure. When properties of defects at dilute concentrations are desired, the - often incompatible - need for large supercells is added to the above functional requirement. We have recently established self-consistent, site-dependent DFT+U and DFT+U+V as promising approaches to address the challenge of simultaneously meeting these requirements. The minimal added cost of DFT+U(+V) compared to a semi-local functional enables the treatment of large supercells, yet the structural and electronic properties relevant for point-defect calculations agree well with hybrid-functionals. We ascribe this to both the self-consistent determination of the Hubbard parameters that leads to an internal consistency of results, as well as the site dependence, which for localized defect states captures chemical changes on multivalent ions around the defect. We will highlight the performance of the method for oxygen vacancies in the perovskite oxides $\mathrm{SrTiO_3}$ and $\mathrm{SrMnO_3}$. In the former self-consistent DFT+U+V leads to an electronic structure of oxygen vacancies that agrees well with that of hybrid functionals, which also translates to similar formation energies that agree well with experiment.

MM 18: Poster Session I

Time: Monday 18:15–20:00 Location: P4

MM 18.1 Mon 18:15 P4

Analysis of polymers and stainless steels by scanning and transmission electron microscopy — •Bernhard Kaltschmidt, Inga Ennen, and Andreas Hütten — Thin Films & Physics of Nanostructures, University of Bielefeld, Bielefeld, Germany

The mechanisms of material aging are investigated to have a better understanding of the durability of materials. The aim of this work was to investigate the molecular changes induced by material aging. We examined polypropylene with different fillers like glass fibers and talcum. Here we analysed the microstructure of polypropylene after etching and heating. The polypropylene samples were freeze fractured and ultramicrotomed in different orientations. The stainless steels examined were: 1.4016, 1.4301 and 1.4510. The effects of pitting corrosion under different chemical environments were analysed. The steel lamellas used for TEM analysis of steel were cut by Focused Ion Beam (FIB). Results from SEM and TEM were compared to determine which technique is best suited for the task.

MM 18.2 Mon 18:15 P4

Detection and characterisation of amorphous silicon nanoclusters in laser-annealed silicon-rich silicon oxide via STEM — •Lukas Richert[1], Christoph Flathmann[1], Tobias Meyer[1], Hendrik Voigt[1,2], and Michael Seibt[1] — [1]IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]currently at Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Low-dimensional silicon such as crystalline or amorphous silicon nanostructures exhibit room-temperature photoluminescence in the visible range, which may lead to low-cost optoelectronic integrated circuits and LED displays. Laser annealing of an amorphous silicon-rich silicon oxide (SRSO) film with laser powers of 40 to 50 mW results in the thermal decomposition of SRSO into silicon and silicon oxide.

As a result of annealing, three distinct morphologies can be identified. Laser damage results in a porous area, surrounded by a silicon nanocrystalline-rich material and, finally, a phase-separated amorphous region consisting of amorphous silicon nanoclusters (aSi-NCs) and silicon oxide. Cross-sectional TEM lamellae are analysed using fluctuation electron microscopy and electron energy loss spectroscopy to investigate the microstructure of the laser-annealed sample and verify the existence of aSi-NCs.

MM 18.3 Mon 18:15 P4

Time and temperature resolved in situ investigation of the metal-induced crystallization of amorphous carbon thin films — •Matthias Krause[1], Daniel Janke[1], Robert Wenisch[1], René Heller[1], David Rafaja[2], and Sibylle Gemming[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden — [2]Institute of Materials Science, TU Freiberg, 09599 Freiberg — [3]Institute of Physics, TU Chemnitz, 09126 Chemnitz

The metal-induced crystallization of amorphous carbon in thin film stacks with Ni was investigated in situ as a function of initial stacking order, temperature and time by Rutherford backscattering spectrometry and Raman spectroscopy. Four different bilayer and triple layer stacks were exposed to heating ramps up to 700 °C. Formation of turbostratic carbon occurred simultaneously with a layer exchange (LE) and was completed during the applied heating ramp up to 700 °C. The temperature resolved measurements allowed the determination of the onset temperatures and transition rates as a function of the annealing temperature and the stacking order. Finally, the activation energy for both LE directions was estimated. In combination with the thermodynamic calculations, this in situ study allows to identify the metal-induced crystallization via wetting and diffusion along grain boundaries, instead of dissolution/precipitation upon annealing as the responsible mechanism for crystallization of amorphous carbon with layer exchange in contact with Ni.

MM 18.4 Mon 18:15 P4

Phase Transformations in TiAl during Selective Laser Melting (SLM) studied by X-ray Diffraction — •Jan Rosigkeit, Peter Staron, Emad Maawad, and Florian Pyczak — Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany

Interest in SLM has dramatically expanded in the last several years, owing to the advantages of additive manufacturing (AM) compared to conventional manufacturing. The possibility to generate complex components just from CAD-data using a layer-by-layer process may reduce production costs, lead times and material consumption. Complex components can be produced without a mold, and structures can be generated that cannot be produced by other techniques. AM attracts strong attention in the area of high performance materials like intermetallic Titanium Aluminide (TiAl) alloys. They represent innovative materials for high-temperature applications in aviation or energy generation, e.g. turbines blades. However, the cyclic heating and cooling during SLM leads to heat treatments of the previous solidified layers changing the phase content and inducing large residual stresses. Therefore, TiAl has so far only been additively manufactured using electron beam melting, which easily facilitates substrate heating to the required temperatures. Nevertheless, SLM of TiAl can also be achieved with sufficient substrate heating. This study focuses on the phase transformations and residual stress build-up as a function of process parameters in order to understand cracking. For this, diffraction measurements with high-energy X-rays were performed in-situ using an SLM chamber developed for use at a synchrotron beamline.

MM 18.5 Mon 18:15 P4

Antiphase domain growth on cubic lattices: a Monte Carlo study — •Ulrike Zweck and Michael Leitner — Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching

The ordering process in binary alloys, following the quench from a disordered state, has a great influence on system properties, such as magnetism or hardness. Describing the atomic ordering process as well as its kinetics accurately is crucial for understanding the correlation of system properties and structural order. The most accessible quantity in measurements, for example in scattering and diffraction experiments, is the structure function $S(k)$.

To give a general model for describing the ordering process and the behavior of antiphase domains (APDs) growing isotropically on crystal structures we investigate systems on cubic lattices via Monte Carlo simulations. We study systems exhibiting two, three or four APDs during the ordering process in the Ising model, the simplest atomistic model, as well as the standard q-state Potts model, which allows us a more abstract view on the ordering process. To describe and compare the growth and coarsening of APDs we exploit the scaling behavior of the pair correlation function as well as its Fourier transform $S(k,t)$ and obtain a scaling factor L for each time step in the ordering process. We define a master curve describing simultaneously the scaled correlation functions as well as their scaled Fourier transforms $S(k)L(t)$ and determine the kinetics of APDs in terms of $L(t)$. Thereby we obtain an explicit and quantitative coupling of length scales in real and reciprocal space.

MM 18.6 Mon 18:15 P4

Analysis of Crystal Defects in Tungsten by Positron Annihilation Lifetime and Doppler-Broadening Spectroscopy — •Vassily Vadimovitch Burwitz[1], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Physik Department E21 and FRM II, TU München — [2]Max-Planck-Institut für Plasmaphysik, Garching bei München

The quantitative analysis of radiation defects in tungsten is important for the safe operation of future nuclear fusion reactions.

Positron annihilation measurements were conducted in order to trace defect evolution through the treatment steps. All tungsten samples studied were cut by spark erosion from the same single-crystal rod with orientation (111), polished mechanically and electro-chemically before annealing at 2300 K under vacuum. One set of samples was irradiated by an MeV electron beam to different fluences, in order to produce Frenkel pairs as the predominant defect type. The other set was quenched from various temperatures close to the melting point in order to freeze in single vacancies at well-defined concentrations. This procedure provides a benchmark for single vacancies, thereby it is possible to determine if other defect types are present too. Positron annihilation lifetime (PALS) and Doppler-broadening spectroscopy (DBS) was performed simultaneously using a Na-22 source with two samples in sandwich geometry. First results are presented showing how different defect types in tungsten can be characterized by a combined analysis of DBS and PALS data.

MM 18.7 Mon 18:15 P4

Optical testing of phase change materials — •Simon von Oehsen, Maximilian Müller, Christoph Persch, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, 52074, Germany

Faster switching enables advances in information storage. The well established phase change materials have proven to be a promising candidate to increase the switching speed of non-volatile memory. Yet, after over two decades of research its kinetics are still not fully understood.

The phase change optical tester (POT) provides the possibilty to measure the reflectivity change during crystal growth in real time over 8 orders of magnitude down to 10^{-8} s. The sample temperature can be tuned by an underlying heater and a laser, whose different heating parameters open up a variety of measures to study phase transformations. It allows the examination of as-deposited material as well as melt-quenched systems. Many phase change compounds are continuously being studied this way.

The power of the employed laser is yet to be transformed to a temperature by simulation and calibration to the heater or differential scanning calorimetry in order to better access, compare and process the data in the well known time-temperature-transition (TTT) diagram.

MM 18.8 Mon 18:15 P4

Glass Dynamics and Crystallization Kinetics of the System GeSe:GeTe — •Maximilian Müller, Julian Pries, and Matthias

Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, 52074, Germany

To optimize the application potential of phase-change materials (PCM) as random access memory switching speed from amorphous to crystalline phase has to be minimized. For a better understanding of the crystallization process of different materials it is important to clarify if crystallization occurs from the undercooled liquid phase or from a glassy phase and would be thereby depending on aging processes.

Because the glass transition of most phase change materials can not be observed in standard differential scanning calorimetric (DSC) measurements, a system of GeSe:GeTe was used to trace the stoichiometry dependence of glass transition from GeSe (non-PCM) for which glass transition is observable to GeTe (PCM) for which it is not. Additionally, ultra-fast DSC and standard DSC were used to explore the interplay of the glass transition and crystallization for heating rates in a range of more than 6 orders of magnitude.

From these data a lower boundary of the glass transition temperature of GeTe could be determined for a wide range of heating rates, especially for the standard glass transition heating rate of 20 K/min. The resulting dataset is also a promising starting point for further studies of glass dynamics and crystallization kinetics of GeTe.

MM 18.9 Mon 18:15 P4

Combining Atom Probe Tomography and Statistical Mechanics: Analysis of the Miscibility Gap in Copper-Nickel — •Marvin Poul, Rüya Duran, Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Deutschland

Although Copper-Nickel alloys are commonly used in technical applications, their alloying behavior at low temperatures is still controversial. Early theoretical and indirect experimental investigations indicated that the phase diagram may contain a miscibility gap. Nevertheless, direct experimental proof is missing due to the slow kinetics at low temperatures.

This work combines thin film Atom Probe Tomography measurements with a novel methodology based on statistical mechanics to extract T_c from histograms of thermodynamically inherent local concentration fluctuations annealed above T_c, i. e. in the region of complete miscibility, to side-step the slow kinetics. The same formalism allows access to relative chemical potential differences between samples with different mean concentration and the excess Gibbs free energy of mixing as a function of concentration, allowing direct approach to a Calphad parametrization.

The approach is showcased using Monte Carlo simulations and Atom Probe Tomography measurements of Copper-Nickel, yielding a T_c appreciably lower than the expected 600 K from current Calphad parametrizations and too low to be practically accessed in experiment.

MM 18.10 Mon 18:15 P4

Experimental investigation of the early stage precipitation reactions in Al-Cu alloys — •Johannes Berlin, Maximilian Gnedel, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg (Germany)

Due to their superior strength to weight ratio heat treatable Al-Cu alloys (2XXX-Series) are widely used particularly in aerospace industry. Although the occurring precipitates in these alloys are well known, the very early stages of formation and transformation mechanisms still are a topic of ongoing research. Transmission electron microscopy is used to investigate the influence of different parameters such as thermal history and additional plastic deformation on early stage precipitation in aluminum. Based on state-of-the-art transmission electron microscopy natural aging in form of growing GP-zones accelerated by excess vacancies can be examined, which was possible before only by diffraction experiments. In addition, DSC and hardness measurements are performed to evaluate the temper state of the specimens. The results are compared to numerical simulations. A better understanding of the precipitate formation mechanisms in these alloys for important future light-weight construction could be tuned more precisely regarding their intended use.

MM 18.11 Mon 18:15 P4

Analysis of grain boundary character and the resulting hardness distribution in High Entropy Alloys — •Lydia Daum, Bengü Tas, Martin Peterlechner, Sergiy Divinskiy, and Gerhard Wilde — Institute of Materials Physics

In this study four and five component alloys, CoCrFeNi and CoCrFeMnNi respectively, were prepared with different heat treatments to analyse their grain boundary character and their microstructures and mechanical properties. Thus, XRD, EBSD, EDX and Vickers microhardness indentation measurements have been carried out. The equiatomic distribution of the alloy components was shown with EDX maps for the polycrystalline alloys. A CoCrFe and a MnNi rich area was identified for the five component alloy which had been annealed at 500°C. An increase in hardness of about 8% was observed after annealing at temperatures between 500°C and 600°C for CoCrFeMnNi and CoCrFeNi, respectively. To compare each hardness value with respect to the grain orientation, a grid of hardness indentations were imprinted onto the sample surface and that surface was subsequently analyzed again by EBSD. Calculating for each hardness measurement the Schmid factor, a correlation between orientation and hardness was observed. Especially indentations in (1 1 1)-planes measured increased hardness values.

MM 18.12 Mon 18:15 P4

Electronic structure and stability studies on random configurations of silicon-germanium carbon alloys — •Willi Roscher[1], Florian Fuchs[2,3,4], Christian Wagner[5], Jörg Schuster[2,3,4], and Sibylle Gemming[4,5] — [1]Leibniz Institute for Solid State and Materials Research Dresden, D-01069 — [2]Fraunhofer Institute for Electronic Nano Systems, D-09126 — [3]Center for Microtechnologies, Technische Universität Chemnitz, D-09126 — [4]Institute of Physics, Technische Universität Chemnitz, D-09126 — [5]Helmholtz-Zentrum Dresden-Rossendorf, D-01328

One important application of silicon-germanium carbon are heterojunction-bipolar transistors (HBTs). Current research aims to reduce the device dimensions, making fluctuations on the atomic scale a serious concern. We therefore study the statistical distributions of the electronic properties in bulk $\mathrm{Si}_{1-x-y}\mathrm{Ge}_x\mathrm{C}_y$. The entire composition range $0 \leq x \leq 1$ including small carbon concentrations is considered. Density functional theory is used in this study.

We demonstrate fluctuations of the band gap, which are in the range of about 10 %. These fluctuations occur in bulk SiGeC on a local scale, and they will become observable in down-scaled devices. Further properties, such as the lattice constant, the formation energy, and the change of Gibbs free energy are studied as well. Entropic contributions decrease the Gibbs free energy of mixed systems, which stabilize SiGeC at room temperature. Finally, local changes of the band gap in an HBT due to a spatially varying germanium concentration are presented.

MM 18.13 Mon 18:15 P4

On the complex structure and phase boundaries in Fe-Al binary alloys — •Subhamoy Char and Dasari Prasad — Department of Chemistry, Indian Institute of Technology Kanpur, UP-208016, India

Although elemental Fe and Al are simple metals in their respective ground states, the solubility of one in another with varying composition leads to a series of intermetallic $\mathrm{Fe}_x\mathrm{Al}_y$ phases consists of wide variation in structure, electronic, magnetic, and mechanical properties. The phases are dressed-up with full of complexities that are often challenged the computations to comprehend the structure-property relationship. This is mostly attributed due to the fact that the structures undergo temperature driven order-disorder phase transformations, thermal vacancies, antisite defects, and ambiguous phase segregation between different Fe-Al phases. Therefore, it is indispensable to correctly model the phase diagram by predicting the Fe-Al structures at finite temperature. While the DFT is more effective in calculating total energies and forces of such alloys, it is computationally quite an arduous task in predicting the structures across the temperature verses the compositional structure state-space of Fe-Al phase diagram. Here, we have adopted a hybrid data-driven, stochastic and evolutionary crystal structure prediction approach coupled to DFT electronic energy calculations to predict thermodynamically viable structural solutions and thereby the Fe-Al phase boundaries are constructed. It is found that the vibrational entropy essentially steers the inexplicable phase segregations in Fe-Al binary alloys.

MM 18.14 Mon 18:15 P4

Analyse und vergleichende Synthese von anodischen Aluminiumoxidschichten auf technischen Aluminiumlegierungen — Ivan Zadyraka, Stefan Ostendorp, Martin Peterlechner und •Gerhard Wilde — Institut für Materialphysik und CeNTech, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, D-Germany

Bauteile aus technischen Aluminiumlegierungen finden in vielen Bereichen Anwendung. Die Oberflächenvergütung mittels Anodisierung stellt hierbei ein wichtiges Mittel dar, um sowohl die mechanische als auch chemische Resistenz der Bauteile zu gewährleisten. Ziel dieser Arbeit ist die Untersuchung vermeintlich vergleichbar oder ähnlich hergestellter Aluminiumoxidcoatings auf verschiedenen Aluminiumlegierungen mit einem Fokus auf den strukturellen und chemischen Eigenheiten dieser Schichten. Mit Hilfe von elektronenmikroskopischen Untersuchungen inkl. EDX-basierter Elementanalysen sollen Korrelationen zwischen mikroskopischen Eigenschaften und der makroskopisch ermittelten chemischen Resistenz der untersuchten Schichten hergeleitet werden. Zum Vergleich wird Rohmaterial der entsprechenden technischen Legierungen in variierenden Oxal- und Phosphorsäure-basierten Elektrolyten unter DC-Potential und potentiostatischen Bedingungen im Labormaßstab anodisiert. Analog zu den kommerziellen Produkten wird anschließend ein Heißwasser-Sealing angewendet. Analysen dieser Coatings zeigen Unterschiede zu kommerziellen und somit gebräuchlichen Schichten auf und erlauben die Diskussion über einen optimierten Herstellungsprozess für solch schützende Aluminiumoxidschichten.

MM 18.15 Mon 18:15 P4

Copper Precipitates in Aluminum Alloys studied by Positron Annihilation Spectroscopy — •Leon Chryssos, Thomas Gigl, and Christoph Hugenschmidt — Physics Department E21 and Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München

Aluminum alloys are an integral part of modern engineering. However, due to its poor welding properties and rigidity, pure aluminum is not suitable for most industry applications. Therefore, most of the shortcomings of pure aluminum can be mitigated by alloying percentage amounts of copper. The formation of copper precipitates in the aluminum lattice introduces strain and, hence, improves rigidity. Due to its, in comparison to Al, greater positron affinity, Cu clusters can be detected in AlCu alloys using Coincident Doppler Broadening Spectroscopy (CDBS). To better understand the precipitation process the Al alloy EN AW-2219 T87 was treated under different conditions ,i.e. samples were prepared using different artificial aging procedures. Afterwards they were analysed using the CDB Spectrometer at NEPOMUC/FRMII of the TU München. With this method it was possible to determine optimal aging parameters for the alloy. A summary of the investigated procedures will be presented, giving an insight into the Cu precipitation process and dissolution of precipitates under different annealing conditions.

MM 18.16 Mon 18:15 P4

DFT characterization of β- and δ- intermetallic Al-Fe-Si phases — •Nebahat Bulut[1], Hanka Becker[2], Andreas Leineweber[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, Germany

The β-Al$_{4.5}$FeSi and δ-Al$_3$FeSi$_2$ phases are known stable phases of Fe-containing Al-Si alloys. Despite the known stoichiometry of the β- and δ- phase the positions of the Al and Si atoms in these Al-Fe-Si intermetallic phases could not be uniquely determined experimentally [1]. Therefore possible positions of Si atoms in these intermetallic phases were investigated using the density functional theory (DFT) code Quantum Espresso, which is based on plane waves and pseudopotentials [2]. For all calculations the PBE exchange-correlation functional has been used.

For both β- and δ- phase different arrangements of Si atoms in the Al-Fe-Si intermetallics were considered. We compare the energies of these arrangements (1) relaxing the atomic positions keeping the unit cell volume constant and (2) fully relaxing atomic positions and unit cell shape and volume. As result we find that arangements where the Si atoms are not nearest neighbours are energetically favored. Further, we analyze the electronic structure and investigate the bonding.

[1] Becker et al., JAC 780:917-929, (2019)
[2] P. Giannozzi et al., J.Phys.Condens.Matter 21, 395502 (2009)

MM 18.17 Mon 18:15 P4

Ab initio opto electronic properties of magnesium silicide alloys — •Juan Guerra, Marcel Giar, Carsten Mahr, Michael Czerner, and Christian Heiliger — Justus Liebig University Giessen, Institut für Theoretische Physik, Giessen, Germany

Due to an increasing interest in the use of environmentally friendly materials for energy conversion, we present a comprehensive ab initio analysis of the opto electronic properties of magnesium silicide materials. These materials have shown an enhancement in the thermoelectric performance when alloyed by Sn as consequence of the convergence of the conduction bands and the reduction of thermal transport. Mg2Si and Mg2Ge have also be shown to be thermodynamically unstable when alloyed by Sn for compositions between the so-called miscibility gap. Our calculations are based on the full-relativistic Green's function Korringa, Kohn and Rostocker (KKR) formalism, within the coherent potential approximation (CPA). We perform total energy calculations to obtain optimal structural properties and relative formation energies to interpret the material's instability. Using the Bloch spectral density function (BSF), we interpolate and map the electronic bands to extract relevant parameters for transport, e.g., band gaps and effective masses within the single parabolic band approximation. We also provide calculations of the contributions to the dielectric function due to direct interband transitions via the joint density of states (JDOS).

MM 18.18 Mon 18:15 P4

Lattice Dynamics of W-Cr Alloys by Ab Initio Calculations — •Michal Farana, Andrzej Piotr Kadzielawa, and Dominik Legut — IT4Innovations, VSB - Technical university of Ostrava, 17.listopadu 2172/15, CZ 708 00 Ostrava - Poruba, Czech Republic

Tungsten alloys are promising candidates to replace the currently favored choice - pure tungsten [1] in the first wall applications in future fusion facilities. The main goal of the alloying of tungsten is to gain additional properties such as self-passivation under accidental conditions [2,3]. According to the W-Cr phase diagram [4], the single solid BCC solution experiences tendency for phase separation within the miscibility gap to reach thermodynamic equilibrium. We applied the Density Functional Theory both within the Special Quasirandom Structure and Virtual Crystal Approximation frameworks to obtain a realistic model of Tungsten-Chromium alloy, with the elastic (via deformation of the crystal) and thermodynamic (via the phonon spectra within the Quasiharmonic Approximation) properties to be compared with experimental data. Based on our results we promote a possible route to enhance both melting temperature as well as the miscibility gap in the Cr-W alloys.

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[2] F. Koch, H. Bolt. **T128**, 100-105 (2007).
[3] M. Vilémová, K. Illková, F. Lukáč. **127**, 173-178 (2018).
[4] W-Cr phase diagram, Bul. of Alloy Phase Diagr. Vol. 5 No. 3 1984.

MM 18.19 Mon 18:15 P4

Computational prediction of solubility limits in selected solid solutions — •Ondřej Fikar and Martin Zelený — Faculty of Mechanical Engineering, Brno University of Technoloty, Brno, Czech Republic

We provide a theoretical study of the phase stability of solid solutions in Al-Ge, Al-Pb, Ag-Au, Ag-Ge and Ag-Pb alloys, in which there are no intermediate phases across the whole composition range. Solubilities of Au, Ge and Pb in Ag and Al were determined using temperature-dependent free energies of pure elements and corresponding Al- and Ag-rich solid solutions obtained from ab initio calculations based on density functional theory. Contributions of vibrational free energy calculated from phonons, electron free energy and configuration entropy were considered. The temperature, at which a solid solution become stable, was estimated from the free energy difference between solid solution and mixture of pure elements. In case of the Al-Ge alloy, quasiharmonic approximation was employed to include also the effect of volume expansion. For this system we employed more precise approach where mixture of Ge and Al-rich solid solution with maximum solubility were considered instead of mixture of pure elements. Predicted solubilities were compared with experimental ones in phase diagrams provided by the CALPHAD method. The results qualitatively agree with experimental observations. However, the exact temperatures at which the solid solutions become stable are underestimated.

MM 18.20 Mon 18:15 P4

Impact of magnetism on the energy of stacking faults in the $C14$ NbFe$_2$ Laves phase — •Ali Zendegani, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The stacking fault energy (SFE) is a key descriptor for predicting plastic deformation mechanisms of materials. In Laves phases basal synchroshear-formed stacking faults (BSSF), which locally transform the hexagonal $C14$ into the cubic $C15$ Laves phase, support the propagation of dislocations. The calculation of the BSSF in $NbFe_2$, however, results in a negative energy, if a ferrimagnetic ground state configuration is used for the *ab initio* supercell. The underlying reason is that ferrimagnetic $C15$ is more stable than ferrimagnetic $C14$ in this system [1].

Considering the very low magnetic ordering temperature of 10 K we, therefore, performed computationally challenging paramagnetic calculations. In this case $C14$ has the lower energy as compared to $C15$. A transfer of this method to the more complex BSSF containing supercells is not yet feasible. Instead, we present an alternative analytical approach [2], which correlates the SFE with the difference of the $C14$ and $C15$ bulk energies and thus allows to determine the energy of the complex BSSF in $NbFe_2$ properly including the magnetic contribution [1].

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MM 18.21 Mon 18:15 P4

Large-scale simulations of plasticity in nanocrystalline Iron — •Hoang-Thien Luu and Nina Gunkelmann — Institute of Applied Mechanics, TU Clausthal, Germany

Shock compression is widely used to investigate the mechanical responses of iron under dynamic loading. It has been long known that α-iron transforms to ϵ-iron under high pressure. Recently, molecular dynamics simulations have shown that plasticity occurs just before the parent phase transforms into ϵ-iron. To provide insights into the interplay of elastic and plastic activities during shocks in iron, we performed atomistic simulations of shock compression of nanocrystalline iron with a mean grain size of 20 nm comprising a total number of 267.5 million atoms. We observed elastic and plastic deformations before the phase transformation takes place. The plastic state is metastable and highly depends on the deformation rate. After a relaxation process of a few picosecond, the structure transforms to a quasi-3D compressed state in which the new phase is stable. The process is ramp time-dependent. In addition, we found that with increasing ramp time of the piston, the period of plasticity is longer.

MM 18.22 Mon 18:15 P4

Electronic and Optical Properties of Bismuthene on a SiC Substrate — •Armando Consiglio and Domenico Di Sante — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

The work focuses on the study of the electronic and optical properties of a material based on a monolayer of Bismuth atoms in an honeycomb structure, known as Bismuthene, supported by an insulating Silicon Carbide (0001) bilayer substrate that stabilizes the system and that contributes to the electronic properties. As the high atomic number of Bismuth atoms leads to an high Spin-Orbit Coupling, and so to large values of the energy gap, this material is promising in the framework of the Quantum Spin Hall systems. Here we show our results based on first principles calculations, obtained via Density Functional Theory and GW methods, and we compare them with experimental results.

MM 18.23 Mon 18:15 P4

Self-consistent implementation of meta-GGA functionals in the (L)APW code Wien2k — •Jan Doumont, Fabien Tran, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

We present a self-consistent implementation of meta-GGA functionals in a full-potential (linearised) augmented plane-wave density functional theory (DFT) code. Because the exchange-correlation (xc) potential is not multiplicative the generalised Kohn-Sham (gKS) formalism was used. To evaluate the energy and potential of the functionals, Libxc was used. We will discuss the novel (compared to a GGA functional) contributions to the matrix elements of the hamiltonian and discuss their implementation. Furthermore we present some convergence and performance tests of the meta-GGAs compared to PBE.

MM 18.24 Mon 18:15 P4

Theoretical Description of Non-linear Processes in magnetic material — •Shalu Rani and Valérie Veniard — École Polytechnique, Institute Polytechnique de Paris, Palaiseau, France

Chromia is an anti-ferromagnetic insulator and an ideal material to demonstrate ultra-fast control of demagnetization at higher speed. Ultra-fast control on magnetic state could have the strong impact on magnetic recording technology.

Second harmonic generation (SHG) is used to study the optical properties of materials. SHG is forbidden in centro-symmetric materials and it is possible to obtain a structural and electronic characterization for these systems. However, the absence of time-inversion symmetry in antiferromagnetic materials leads to new contributions in second harmonic generation, thus revealing the arrangement of spins in the solid. SHG becomes a powerful tool to study of ultra-fast demagnetization processes. Chromia is centrosymmetric, but SHG occur because symmetry broke due to the spin.

There are few satisfactory theoretical descriptions for SHG in magnetic materials, since spin-orbit coupling, electron-electron interactions and local field effect must be treated on the same footing. The project is to calculate the Second order response function of chromia using Time-Dependent Density Functional Theory, and taking into account the many-body effects through an exchange-correlation kernel derived from the Bethe-Salpeter equation (BSE) for the linear response.

Results will be shown for the linear response, the GW corrected band gap for the Chromia and for the BSE calculations

MM 18.25 Mon 18:15 P4

Ab initio studies on NbO_2 — •Kathrin Kulmus, Sibylle Gemming, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz

The insulator-metal transition (IMT) of niobium dioxide occurs at T_c = 1080K with changing the crystal structure. It is found experimentally[1] as well as theoretically[2], that NbO_2 behaves like a one-dimensional conductor in its metallic phase. Regarding excitonic effects, we analysed the dielectric function, the partial density of states and the bandstructure (fat bands) in an all-electron ab-initio calculation, each directionally resolved. We further examined the recently found photoinduced IMT at temperatures below T_c[3], i.e. the separation of the thermal and the electronic phase change.

The all-electron DFT code Questaal[4] was employed for the calculations; we acknowledge many valuable discussions with the developer team.

[1] G. Bélanger et al., Can. J. Phys. **52**, 2272(1974)
[2] A. O'Hara et al., J. Appl. Phys. **116**, 213705(2014)
[3] R. Rana et al., Phys. Rev. B. **99**, 041102R(2019)
[4] www.questaal.org

MM 18.26 Mon 18:15 P4

Towards all-optical spectroscopy of ordered and disordered phononic crystals — •Tobias Claus, Sina Ludewig, and Henning Ulrichs — I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

On this poster we report on our recent progress regarding the conceptual realization, fabrication and optical spectroscopy of disordered and ordered phononic metamaterials. Besides applications in acoustics and heat conduction, such materials can generally be used as macro- to nanoscale toy models for physical phenomena based on wave interference. Note that topological spectral properties are nowadays of great scientific interest mainly regarding electronic structure. But also bosonic excitations like magnons and the here addressed phonons can acquire unconventional properties like localization due to symmetry breaking [1] or due to disorder-induced omnidirectional band gaps. [2] Here, we present our design strategy for metamaterials targeting elastic dynamics from the MHz to GHz spectral range. This strategy is based on FEM modelling of the sample and of the finally envisaged all-optical pump-probe experiment. Secondly, we discuss our experimental setup and first measurements on a sample structured by the focussed ion beam experimental technique. We acknowledge financial support by the DFG within the SFB 1073.

MM 18.27 Mon 18:15 P4

Atomistic study of the influence of oxide shell layers on the material properties of aluminum nanowires — •Hoang-Thien Luu[1], Yudi Rosandi[2], and Nina Gunkelmann[1] — [1]Institute of Applied Mechanics, TU Clausthal, Germany — [2]Department of Geophysics, Universitas Padjadjaran, Indonesia

For materials with high oxygen affinity, oxide layers will significantly change the material properties. At aluminum surfaces, an oxide layer may form in seconds, even under vacuum conditions. Recent studies show that thin amorphous oxide shell layers on aluminum surfaces significantly change the responses of the material. However, the relations between the thickness of the oxidized layer, the temperature and the mechanical response of nanowires have not been investigated intensively. In this study, we use a ReaxFF potential to analyze the influences of oxide shell layers on the material responses of the nanowires under uniaxial loading at different strain rates. We conduct simulations within a wide range of strain rates and temperatures varying between 10K and 500K. The Al-O interface leads to an increased defect nucleation rate at the oxide interface preventing localized deformation.

MM 18.28 Mon 18:15 P4

Investigation of electrostatic and elastic grain interactions in ferroelectric ceramics using the self-consistent mesoscopic switching model — •Ruben Khachaturyan[1], Anna Grünebohm[1], and Yuri Genenko[2] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum — [2]Institute of Materials Science, Technische Universität Darmstadt

The self-consistent mesoscopic switching model simulates polarization kinetics of polycrystalline ferroelectrics taking into account electrostatic interactions [1]. The model is now improved to take into account elastic interactions between grains. This improvement allows for polarization and strain kinetics description taking into account local strains and electric fields. Having a switching barrier as one of the input parameters the model promises to become a bridge between polycrystalline materials and atomistic simulations.

[1] **Correlated polarization-switching kinetics in bulk polycrystalline ferroelectrics. II: Impact of crystalline phase symmetries**, R. Khachaturyan, Y.A. Genenko,*Physical Review B.*, **98(13)**, 134106, (2018)

MM 18.29 Mon 18:15 P4

Impact of pressure on bulk diffusion in TiN: a combined ab initio and molecular dynamics study — •Ganesh Kumar Nayak[1], Ilia Ponomarev[2], Paolo Nicolini[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700, Leoben, Austria — [2]Department of Control Engineering - K335, Faculty of Electrical Engineering, Czech Technical University in Prague, Karlovo náměstí 13, 121 35, Prague 2, Czech Republic

Cutting tools protected with hard coatings have been successfully employed in the industry for almost 50 years. In our project, we investigate Ti(Si)VN nanostructured coatings with the aim to control the formation of V2O5 surface oxide acting as a solid lubricant in order to extend the lifetime of cutting tools. In the present work, we report on state-of-the-art DFT and Molecular Dynamics calculations of diffusion barrier for V and Ti in the crystalline TiN matrix. Special attention is paid to the impact of pressure on the diffusion properties, an effect experimentally relevant since the physical-vapor deposited coatings often exhibit compressive stresses. Interestingly, the preliminary results show no significant impact of pressure on the barrier heights obtained using the nudged-elastic-band method. Detailed analysis of these results as well as discussion of different diffusion scenarios (pathways) will be presented.

MM 18.30 Mon 18:15 P4

Calorimetric Study of Low Melting Eutectics in Chlorine-induced High Temperature Corrosion Environment — •Sophie Winkler, Sebastian Pentz, and Ferdinand Haider — Chair of Experimental Physics I, University of Augsburg, 86135 Augsburg

Waste incineration power plants provide an energetic usage of the produced heat by thermal composition. Complex systems in the exhaust stream are used for the heat extraction at prevalent temperatures of 400–600 °C. These steel pipes are exposed to the flue gas and therefore subject to a high degree of corrosion. The main damage is caused by the chlorine induced high temperature corrosion. Sulfation reactions of the sulfur dioxide with solid alkali chlorides in the flue steam occur which results in a release of chlorine or chlorine compounds in close proximity of the metallic components like superheaters or boiler walls. The released Cl_2 or HCl attack the iron under formation of $FeCl_2$ or $FeCl_3$ leading to a massive removal of the steel material.

The resulting deposits of the steel pipes are then subjected to different methods of thermal and elemental analysis to determine the composition and chemical reactions happening in the corrosion process. Using Differential Scanning Calorimetry, it is possible to construct the phase diagrams of the participating sulfates ($CaSO_4$, K_2SO_4, Na_2SO_4) and to analyse the occurring low melting eutectics that accelerate the corrosion process.

MM 18.31 Mon 18:15 P4

Study of the evaluation of NanoBeam Electron Diffraction Patterns from Bulk Metallic Glasses — •Manuel Lindenblatt, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

An approach to obtain knowledge about the properties of a material is to analyze its structure with diffraction experiments such as in a transmission electron microscope (TEM) done with electron diffraction. Using these experiments to evaluate the structure of a metallic glass proves to be a challenge, since no long range order (LRO) is available. However, the structure of glasses may be characterized by the specific medium range order (MRO) that is present. One possibility to analyze the MRO to evaluate a nanobeam electron diffraction pattern (NBDP) concerning the radial distribution function (RDF).

With the sample being a bulk metallic glass (Vitreloy105, $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ in at%) the focus of the present work is on analyzing the MRO structure of a shear band via obtaining the NBDP (by [1]). This task was approached for each relating parameter individually at first. One significant improvement done by this work is a method to find reliable and reproducible center coordinates for any elliptical undistorted single NBDP. Another contribution relates to the measured background intensity. This work discusses the physical meaning of the parameters relating to the obtained RDFs and discusses also the reliability of information obtained through the RDF analysis concerning the real-space structure of glasses.

[1] S. Hilke et al, Acta Materialia, 171:275-281, 2019.

MM 18.32 Mon 18:15 P4

Investigations on the relaxation of metallic glasses using fast scanning calorimetry — •Maximilian Demming[1], Mark Stringe[1], Martin Peterlechner[1], Gerhard Wilde[1], and Benedikt Bochtler[2] — [1]IMP Uni Münster — [2]LMW Uni Saarland

During isothermal annealing below the glass transition, all glasses, and thus also metallic glasses, show relaxation effects that resemble the underlying trajectory in phase space towards metastable equilibrium. Using fast scanning calorimetry (FSC) it becomes feasible to investigate such phenomena over a wide range of rates and at very high controlled heating or cooling rates. The tremendous advantage of FSC in comparison to a conventional differential scanning calorimeter (DSC) is, that here one can reach cooling and heating rates up to several 10000 K/s, which makes in-situ quenching possible. Another advantage is that a large number of measurements can be performed in small time intervals. This makes the FSC quite interesting for experiments in thermic cycling with controlled heating and cooling rates. One special method is the so-called cryogenic cycling, which means, that a sample is periodically quenched and reheated between room and a cryogenic temperature. According to literature, this treatment, that has been termed as *cryogenic rejuvenation* could lead to markedly changed properties of the metallic glass. The materials investigated here are AuCuSiAg and PdNiS due to their low glass transition temperature and melting point. Here different relaxation states achieved by in-situ quenching via FSC are examined and compared to the relaxation behavior observed at conventional rates.

MM 18.33 Mon 18:15 P4

Investigating the short-range order (SRO) of glassy $Ge_{15}Te_{85}$ and GeSe obtained by TEM diffractometry — •Christian Stenz, Julian Pries, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany

In contrast to the crystalline phase, in the amorphous glassy and undercooled-liquid phase atoms show no long-range order and have no periodic structure. Still, atoms in amorphous solids exhibit a certain short-range order (SRO), which can be inferred from diffractometry. Here, transmission electron microscopy (TEM) is utilized in order to acquire selective area electron diffraction (SAED) patterns of as-deposited amorphous $Ge_{15}Te_{85}$ and GeSe. The 2D diffraction patterns acquired are circularly integrated to obtain 1D diffraction profiles. From these diffraction profiles the pair distribution functions (PDFs) are calculated using *SUePDF* providing insight on the SRO. After background substraction, algebraic redefining and normalization, the PDF is obtained by a Fourier transformation of the 1D diffraction pattern. The PDFs are compared to the expected atomic distances of the crystalline phase by a *MATLAB* program, which outputs the corresponding PDF computed from the unit cell.

MM 18.34 Mon 18:15 P4

Effects of annealing and thermal history of glassy materials — •Alexander Heinrich, Julian Pries, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany

The relaxation dynamics of glassy materials can vary dependent on its thermal history and of the material itself. To understand structural relaxation dynamics more, this process is simulated according to Hodge and Berens. They published their simulating scheme as early as 1981. This simulation uses the expression of Tool Narayanaswamy Moynihan (TNM). This simulation numerically solves the TNM-equation of the fictive temperature T_f for discrete temperature steps. Thereby the normalized heat capacity is calculated by deviating the fictive temperature by temperature. By reproducing this simulation and results of Hodge and Berens, the simulation can be used to simulate the cooling and heating cycle of a glassy material. The simulation enables the prediction of glass dynamics close to the glass transition for different thermal histories.

MM 18.35 Mon 18:15 P4

Signatures of quasiparticle transport in excitonic insulator candidate: Ta_2NiSe_5 — •Yuan-Shan Zhang[1], Jan Bruin[1], Yosuke Matsumoto[1], Masahiko Isobe[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany — [3]Department of Physics, Univerisity of Tokyo, Japan

Ta_2NiSe_5 is a narrow gap semiconductor which is electronically quasi-one-dimensional and undergoes a transition to an excitonic insulator at T_c=328K[1], where the electron-hole pairs condense into a many body ground state. Thermal conductivity is a useful probe for the quasiparticle states as well as the relevant phonons in excitonic insulators.

Here, we present the temperature dependence of thermal conductivity $\kappa(T)$ of single crystals of Ta_2NiSe_5 around the transition temperature, measured along both parallel and perpendicular to the quasi-one dimensional chain direction. We observed a clear anomaly in $\kappa(T)$ at T_c: a kink followed by a raid decrease below T_c for the chain direction and a pronounced dip for the perpendicular to the chain direction.

We argue that, while the former originates predominantly from the quasi-particle contribution, the latter represents the phonon contributions scattered by the shear-mode soft phonons coupled strongly to the excitonic state.

[1] Y. F. Lu et al. Nat. Commun., **8** 14408(2017)

MM 18.36 Mon 18:15 P4

Monte Carlo simulation of the energy distribution in laser-irradiated solids under the influence of a magnetic field — •Xavier del Arco, Julia Amann, Pavel N. Terekhin, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Strasse 46, 67663 Kaiserslautern, Germany

The complex phenomenon arising after irradiation of a solid with ultrashort laser pulse is studied using a Monte Carlo simulation. Two possible electron interactions are considered: inelastic scattering and impact ionization. The influence of the external homogeneous magnetic field on the energy exchange between the electron and lattice subsystems is investigated. The results of this simulation contain the information about the evolution of the electron density, electron and lattice energy distributions. The developed approach can be used to study the influence of the magnetic field on the energy deposition and develop optimal strategies to improve ablation processes in solids.

MM 18.37 Mon 18:15 P4

Interdiffusion and atomic mobility in Mo-Zr and Mo-Nb-Zr bcc phase alloys — •Baixue Bian[1], Yong Du[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Gemany — [2]State Key Laboratory of Powder Metallurgy, Central South University, 410083 Changsha, China

Accurate kinetic characteristics of refractory alloys are critical for understanding and tuning the phase transformation and microstructure evolution during homogenization and precipitation. In this work, the diffusion couple technique, Bltzmann-Matano and Matano-Kirkaldy methods were applied to measure the interdiffusion coefficients of bcc phase Mo-Zr binary alloys and Mo-Nb-Zr ternary alloys at 1423-1523 K, respectively. Subsequently, on the basis of the presently obtained interdiffusivities together with the thermodynamic descriptions for bcc Mo-Nb-Zr system, the atomic mobility parameters of Mo, Nb and Zr elements were assessed by means of DICTRA software package. Moreover, the comprehensive comparisons between the experimental diffusion properties (i.e., interdiffusivities, composition profiles, and diffusion paths) and the calculated /model-predicted data due to the present atomic mobilities were conducted in order to verify the reliability of the mobility values. The present atomic mobilities for bcc Mo-Nb-Zr system are shown to provide the accurate interdiffusivity matrix over a wide composition range.

MM 18.38 Mon 18:15 P4

Investigation of Hydrogen Isotopologue Sorption in Ti/Pd Films — •Sonja Schneidewind[1], Sebastian Vetter[1], Christian Goffing[1], Max Aker[1], Marco Langer[3], Andreas Fleischmann[2], Loredana Gastaldo[2], Andreas Reifenberger[2], and Magnus Schlösser[1] — [1]IKP, KIT, Karlsruhe, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg, Germany — [3]ITEP, KIT, Karlsruhe, Germany

Certain metals can solve hydrogen isotopes in their lattice structure and can subsequently form metal hydrides. Out of these materials, Ti has one of the lowest dissociation pressures which allows for quasi-irreversible hydrogen isotope capture. However, the Ti surface tends to form an oxide layer in air which acts as effective permeation barrier. The oxidation can be prevented by a thin Pd film on top allowing for gas permeation through the Pd layer into the Ti getter. This technique can be used to build effective passive hydrogen isotopologue pumps or by employing the radioactive isotopologue, tritium, one can build dedicated radioisotope heat sources, e.g. for calibration purposes.

We perform sorption experiments by using a quartz crystal micro balance with nanogram resolution to determine the dependence of absorbed gas amount and durability of absorbed gas in Ti/Pd films on loading parameters. Films coated on QCMs are exposed to hydrogen isotopologue gas. XRD and resistance measurements are used to study phase transformations and to verify the absorbed gas amount. The sorption of tritium by the films is investigated by Beta-Induced X-Ray Spectrometry combined with simulations using GEANT4.

MM 18.39 Mon 18:15 P4

Nanoscale heat transport in heterostructures — •Jan-Etienne Pudell[1], Marc Herzog[1], Alexander von Reppert[1], Gregory Malinowski[3], Matthias Rössle[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Institut Jean Lamour, Université Lorraine, Nancy, France

The transport of heat (or energy in general) in nanoscopic heterostructures is of great interest on a fundamental as well as a technological level, e.g. in the context of thermal management in devices or heat-assisted magnetic recording. In metal heterostructures, heat can be conducted by electrons, which are in- or out-of-equilibrium with lattice vibrations. Using time-resolved x-ray diffraction, we investigate the thermal transport through a 100 nm Cu layer sandwiched by thin Pt and Ni films on a glass substrate on picosecond time scales after femtosecond laser excitation. A time-dependent diffusive transport model accurately reproduces our experimental data and thus verifies the efficient transport channel from the laser excited Pt-layer to the Ni-layer via hot electrons. The results imply dominant diffusive instead of ballistic electron transport.

MM 18.40 Mon 18:15 P4

Synthesising high-T_c hydrides for the electrical transport measurements — •Takaki Muramatsu[1], Israel Osmond[1], Owen Moulding[1], Jonathan Buhot[1], Oliver Load[2], and Sven Friedemann[1] — [1]School of Physics, University of Bristol, UK — [2]School of Earth Science, University of Bristol, UK

A series of high-T_c superconductors (LaH_x, YH_x, and ThH_x) have been reported in hydrogen-rich hydrides under extreme high pressures since 200 K superconductivity was discovered in H_3S in 2015 [1-6]. The hydrides are synthesised under high pressure above 100 GPa by using laser-heated diamond anvil cell (DAC) technique and the superconducting transitions are detected by electrical transport measurements in the DACs. However, these techniques are established only in a limited number of groups so far. Therefore, we pursued to acquire the experimental techniques to observe the high-T_c superconductivity of the hydrides. Recently we successfully synthesised the hydrides (H_3S, LaH_x and YH_x) and observed the resistance drops in the temperature dependence of electrical resistance. The resistance drops were confirmed to be superconducting transitions as the temperatures of the drops shift to lower temperature with applied magnetic field. Our study now focuses on synthesising high quality samples and observing zero resistance of the superconductors.

MM 18.41 Mon 18:15 P4

The study of non-linear Hall effect via semiclassical theory — •Botsz Huang[1] and Ching-Hao Chang[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan 701, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan

Ordinary Hall effect is driven by an applied magnetic field that provides Lorentz force on a charge carrier and thus leads to charge accumulation perpendicular to the current direction. While anomalous Hall effect occurring in magnetic materials does not require any external magnetic field. It is driven by the Berry curvature that acts an effective magnetic field in momentum space. Based on the mechanics of anomalous Hall effect, non-linear Hall effect due to Berry curvature fluctuation is predicted and also observed in non-magnetic material without any magnetic field. In this talk, a numerical approach solution is presented to study the non-linear Hall effect driven by the magnetic field. The equation of motion of electron is

$$\dot{\mathbf{r}} = -\frac{1}{\hbar}\frac{\partial \mathcal{E}(\mathbf{k})}{\partial \mathbf{k}} + \mathbf{k}\times\boldsymbol{\Omega}(\mathbf{k})$$

$$\hbar\dot{\mathbf{k}} = q\Big(\mathbf{E}+\mathbf{v}\times\mathbf{B}\Big)$$

based on the semi-classical transport theory. According to the equation of motion, the test particle method is employed to trace particle trajectories and to determine the transportation. This work opens a new avenue to investigate the transport in semiclassical region and establishes a connection between ordinary Hall effect and non-linear Hall effect.

MM 18.42 Mon 18:15 P4

Thermal conduction in epitaxial $\mathbf{LaMnO_3/SrMnO_3}$ superlattices — •Daniel Metternich[1], Dennis Meyer[1], Roland Potthast[1], Jan-Phillip Bange[1], Marius Keunecke[1], Robert Gruhl[1], Vladimir Roddatis[2], Vasily Moshnyaga[1], and Henning Ulrichs[1] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Helmholtz-Zentrum Potsdam Deutsches GeoForschungsZentrum

We report on experimental and theoretical investigations of the thermal conduction in $LaMnO_3$ (LMO) / $SrMnO_3$ (SMO) epitaxial superlattice structures, grown by metal-organic aerosol deposition (MAD).

The thermal conductivity of our samples is measured with a transient thermoreflectivity setup - a method that uses a pulsed laser to heat the sample whilst a continuous wave laser measures the surface reflectivity (TTR), and thereby the surface temperature in the time domain. A comparison between samples of different periodicities and LMO/SMO-ratios in particular reveals an unexpected behaviour of the contribution of LMO to the thermal conduction: In single LMO films we find a thermal conductivity close to the amorphous limit, whereas when integrating the LMO into a superlattice, its contribution to the conductivity strongly increases. We relate this finding to a structural modification of the LMO layers in the superlattice.

In addition, we compare our findings with theoretical first-principles calculations regarding the structural configuration of the multi-layered system as well as the phononic contributions to the heat transfer. We acknowledge financial support by the DFG within SFB 1073.

MM 18.43 Mon 18:15 P4

Synthesis and luminescence properties of Ca(1-x)Eu(x)AlSiN3 — Norovsambuu Tuvjargal[1], Chao Kefu[2], Ojied Tegus[2], and •Jav Davaasambuu[1] — [1]Department of Physics, National University of Mongolia, Ulaanbaatar, Mongolia — [2]Inner Mongolia Key Laboratory for Physics and Chemistry of Functional Materials, Inner Mongolia Normal University, Hohhot, China

Ca(1-x)Eu(x)AlSiN3 is currently one of the best known red-emitting materials for LED applications. We will present the experimental results of structural and optical properties of Ca(1-x)Eu(x)AlSiN3 samples. Ca(1-x)Eu(x)AlSiN3(x=0.02, 0.04, 0.06, 0.08, 0.1) samples were successfully synthesized by the high-temperature solid state reaction method. The structure and luminescence properties of samples were investigated by x-ray diffraction and spectroscopic measurements. The Ca0.96Eu0.04AlSiN3 sample shows the strongest red fluorescence emission peak at 670nm under the excitation wavelength of 450nm.

This work has been done with financial support of the Mongolian Foundation for Science and Technology.

MM 19: Invited talk Löffler

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

Invited Talk MM 19.1 Tue 9:30 BAR 205

Ultrafast calorimetry: studying phase transitions in slow motion — •Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland

Studying the details of phase transitions and metastable phase formation is generally difficult for metallic materials because of their rapid nucleation and growth kinetics. Bulk metallic glasses (BMGs), on the other hand, show very sluggish crystallization kinetics. By applying ultrafast differential scanning calorimetry to slowly transforming BMG-forming systems at heating and cooling rates of up to 10^5 K/s, we are able to determine phase transitions more or less in slow motion. This allows us to discover new phase transition pathways, such as solid-state phase transitions that occur via intermediate melting [1]. An important experimental strategy that can in particular be realized via ultrafast calorimetry is to interrupt rapid cooling after (metastable) phase formation and then to "up-quench" the frozen structure via rapid heating. Via surpassing the metastable-to-stable solid phase transition, the formed metastable phase can thus be fully melted, with the possibility of measuring its thermophysical properties such as temperature and enthalpy of melting [2]. We are thus able to discover hidden transient phases, determine the stochastics of nucleation [3], and construct energy-temperature diagrams for metastable phases, with the final aim of constructing complete metastable phase diagrams.

[1] S. Pogatscher et al., *Nature Comm.* **7**, 11113 (2016).

[2] G. Kurtuldu, K. Shamlaye, J. F. Löffler, *PNAS* **115**, 6128 (2018).

[3] J. E. K. Schawe and J. F. Löffler, *Nature Comm.* **10**, 1337 (2019).

MM 20: Topical Session: Interface-dominated phenomena - Diffusion

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

Topical Talk MM 20.1 Tue 10:15 IFW A

The early stage of reactive interdiffusion in the Cu-Al system investigated by in-situ TEM — •Xavier Sauvage[1], Florent Moisy[2], and Eric Hug[2] — [1]Groupe de Physique des Matériaux, UMR CNRS 6634, University Rouen Normandy, France — [2]CRISMAT, University Caen Normandy, France

The early stage of the reactive interdiffusion in the Al/Cu system was investigated by in-situ TEM at 350°C and 300°C. Original Al/Cu interfaces were created by a purely mechanical process using co-deformation at room temperature by drawing. During the reactive interdiffusion three IMCs were detected: Al2Cu and AlCu grew in the Al side and the Al4Cu9 in the Cu side. Systematic comparisons with ex-situ annealed samples and with regions out of the electron beam proved that there was no significant artefact (thin foil or beam effect). Although GBs may act as fast diffusion path, no preferential growth of IMC along these defects could be observed. The mean growth rates of all IMCs follow a classical parabolic law indicating that the kinetic of the transformation is controlled by diffusion mechanisms. A strong deviation was observed however in the early stage of the reaction. Nanoscaled Mg2Si particles located in the Al phase strongly interact with the transformation front. It leads to large fluctuations of the velocity of interphase boundaries at the nanoscale. The pinning effect in connection with change in local concentration gradients and driving forces will be discussed.

MM 20.2 Tue 10:45 IFW A

Influence of atomic interaction on grain boundary self-diffusion in binary solid solutions — •Vladimir A. Esin — Centre des Matériaux, MINES ParisTech, PSL University, France

Atomic interaction of solute atoms with solvent ones has been considered to be of the major responsibility for the effect of solute on grain boundary self-diffusion. It is supposed that during diffusion process the diffusing solvent atoms form atomic complex with solute atoms at grain boundary with the formation of chemical bonds [1,2]. A description of solvent GB diffusion is then given for both B- and C-regimes.

Using such an approach, a new equation for the dependence of solvent GB diffusion coefficient on solute bulk concentration is derived for the systems with simple atomic attraction in GB. Theoretical results predict non-linear dependence of solvent GB diffusion coefficient on solute bulk content, which is in agreement with earlier published experimental data regarding the ease of grain boundary diffusion in alloys of different chemical compositions. More importantly, the equation deduced permits to evaluate, on one hand, the characteristics of solute GB segregation from solvent GB diffusion measurements and, one the other hand, GB diffusion coefficient in pure solvent. Such a numerical data analysis for Fe-Sn system is in agreement with experimental results.

[1] V. Esin, B. Bokstein and A. Rodin, Defect Diffus. Forum 309-310 (2011) p. 29.

[2] V.A. Esin and B.S. Bokstein, Acta Mater. 60 (2012) p. 5109.

MM 20.3 Tue 11:00 IFW A

Development of a copper–nickel embedded-atom potential for a systematic study of grain boundary segregation and grain boundary formation energy — Felix Fischer and •Sebastian Eich — Institut für Materialwissenschaft, Universität Stuttgart

In this atomistic study [1] on the copper–nickel system, a new embedded-atom alloy potential between copper and nickel is fitted to experimental data on the mixing enthalpy. The resulting phase boundaries of the new potential are in very good agreement with a recent CALPHAD prediction. Using this new potential, a high angle symmetrical tilt $\Sigma 5$ grain boundary (GB) is chosen for a systematic investigation of equilibrium GB segregation in the semi-grandcanonical ensemble at temperatures from 400 K to 800 K. Applying thermodynamically accurate integration techniques, the GB formation energy is calculated exactly and as an absolute value for every temperature and composition.

Eventually, the thermodynamically unambiguous GB solute excess Γ, obtained from the simulations, is fitted to a recently proposed analytical model for interface segregation [2]. Based on a composition-dependent model curve of the energy of segregation, the solute excess Γ can be described excellently over the entire composition range for all investigated temperatures.

[1] F. Fischer, G. Schmitz, and S. M. Eich, Acta Mater. 176, 220 (2019)

[2] T. Krauß, S. M. Eich, Acta Mater. (submitted)

MM 20.4 Tue 11:15 IFW A

Mechano-chemical coupling by microstructure evolution of an Al-Sc-Zr-based alloy — •Bengü Tas, Friederike Emeis, Vladislav Kulitcki, Martin Peterlechner, Gerhard Wilde, and Sergiy V. Divinski — Institute of Materials Physics, University of Münster, Münster, Germany

Al-based alloys are attractive materials for aerospace applications owing to their low density, sufficient weldability and superior strength at room temperature. Severe plastic deformation via equal channel angular pressing at 300°C for 12 passes is applied on a technical AA5024 Al-based alloy in order to produce an ultrafine grained microstructure (UFG) with different types of micro- and nano-precipitates, basically Al_6Mn and $Al_3(Sc,Zr,Ti)$. Heat treatments under different external stress fields are subsequently applied using a universal testing machine. The impact of the stress state (pure shear, uniaxial compression or stress-free annealing) on the microstructure evolution including relaxation of residual strains and precipitation is investigated. The mechano-chemical coupling on different scales is examined with a focus on the evolution of core-shell $Al_3(Sc,Zr,Ti)$ particles. Pure shear results in relatively large grains with a bimodal size distribution, in contrast to smaller, homogenously distributed grains under uniaxial compression. The impact of the stress state on nano-precipitate evolution is elucidated using analytical and high-resolution transmission electron microscopy.

MM 21: Transport - Ions and Electrons

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

MM 21.1 Tue 10:15 IFW B

Site energy distribution of sodium ions in a sodium rubidium borate glass — •Martin Schäfer, David Budina, and Karl-Michael Weitzel — Universität Marburg, Fachbereich Chemie

A charge attachment induced transport experiment [1] has been conducted on a Na^+ and Rb^+ containing glass employing an external Rb^+ ion beam. Native Na^+ ions are replaced by external Rb^+ ions giving rise to a pronounced concentration depth profile as measured by time-of-flight secondary ion mass spectrometry. From the theoretical analysis of this concentration profile a unique site energy distribution (SED) of mobile Na^+ ions in the glass is derived [2]. The full width at half maximum of the populated part of this SED is 0.32 eV. The mechanism involves Na^+ sites being vacated top-down and being filled by Rb^+ also top down. Therefore, the Fermi energy of Na^+ ions decreases with ongoing experiment, while that of the Rb^+ ions stays constant. Agreement between experiment and the Nernst-Planck-Poisson theory for describing the transport is reached by assuming that both the migration and the chemical diffusion driven contribution to the total flux depend on the local concentration. [1] M. Schäfer, K.-M. Weitzel, Materials Today Physics, 5, 12-19, (2018). [2] M. Schäfer, D. Budina, K.-M. Weitzel, Phys. Chem. Chem. Phys, in press (2019).

MM 21.2 Tue 10:30 IFW B

Quantum Paracrystalline Shear Modes in Metals — •Jun Yong Khoo[1], Falko Pientka[1], Po-Yao Chang[1,2], and Inti Sodemann[1] — [1]Max-Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan

Unlike classical fluids, a quantum Fermi liquid can support a long-lived and propagating shear sound wave, reminiscent of the transverse sound in crystals, despite lacking any form of long-range crystalline order. This mode is expected to be present in moderately interacting metals where the quasiparticle mass is renormalised to be more than twice the bare mass, but, it is hard to excite and detect because it does not involve charge density fluctuations, in contrast to the conventional plasma mode. In this work we propose a strategy to excite and detect this unconventional mode in clean metallic channels. We show that the shear sound is responsible for the appearance of sharp dips in the AC conductance of narrow channels at frequencies matching the shear sound dispersion. The liquid resonates while minimizing its dissipation, a behavior characteristic of the sliding crystal. Ultra-clean 2D materials such as graphene, $PdCoO_2$, and MgZnO/ZnO 2DEGs are therefore particularly promising platforms to discover the shear sound.

MM 21.3 Tue 10:45 IFW B

Curve graphene systems to create new Hall-like effects in zero magnetic field — •Ching-Hao Chang[1,2], Sheng-Chin Ho[1], Yu-Chiang Hsieh[1], Shun-Tsung Lo[1], Botsz Huang[1], Thi-Hai-Yen Vu[1], Carmine Ortix[3,4], and Tse-Ming Chen[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan 701, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung Univer- sity, Tainan 701, Taiwan — [3]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, Princetonplein 5, NL-3584 CC Utrecht, Netherlands — [4]Dipartimento di Fisica E. R. Caianiello, Universita Salerno, IT-84084 Fisciano, Italy

In this talk, I will show that Hall-like effects can be created in graphene systems by using curved geometry instead of applying an external magnetic field. We theoretically establish that non-trivial band structure with valley-orbital splitting can be designed in a bilayer graphene (BLG) by corrugating it. This band structure finally generates the transverse resistivity in both linear response and nonlinear response regimes. Our theoretical calculations well address experimental observations qualitatively and quantitatively. This new approach based on tailoring 2D-material geometry opens a new platform to design the band structure to host new transport properties.

MM 21.4 Tue 11:00 IFW B

Quantitative analysis of non-radiative relaxation processes in luminescent borate glass by infrared thermography — •Nils J. Ziegeler[1], Peter W. Nolte[2], and Stefan Schweizer[1,2] — [1]Department of Electrical Engineering, South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest, Germany — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest, Germany

Lanthanide-doped borate glasses represent an interesting class of luminescent materials. Though these systems offer high photoluminescence quantum efficiency (QE) values, a significant part of the excitation power is converted to heat due to unavoidable non-radiative relaxation processes. In this contribution, the amount of generated heat is estimated from infrared thermography investigations. For this, the glass sample's surface temperature is monitored under continuous optical excitation. To obtain the volumetric heat rate, the spatially resolved temperature data are analysed on the basis of the partial differential heat equation. Experiments on barium borate glass with different lanthanide doping concentrations are performed. A comparison with optical measurements shows that the approach to determine the QE indirectly by estimating the amount of non-radiative relaxation processes is very promising and particularly interesting for QE measurements at high temperatures.

MM 21.5 Tue 11:15 IFW B

Investigation of the universal scattering rate in PdCrO2 by high energy electron irradiation — •Elina Zhakina[1,3], Philippa McGuinness[1,3], Seunghyun Khim[1], Veronika Sunko[1], Andrew Mackenzie[1,3], and Marcin Konczykowski[2] — [1]Max Planck Institute for Chemical physics of solids, Dresden, Germany — [2]Laboratoire des Solides Irradies, Ecole Polytechnique, Palaiseau, France — [3]School of Physics and Astronomy University of St Andrews, North Haugh St Andrews, Scotland

PdCrO2 belongs to the delafossite family of extremely pure triangular lattice metals. The CrO2 layers are Mott insulating, and order antiferromagnetically below 37.5K. The resistivity of PdCrO2 is linear in temperature above 150 K. This is in contrast to the non-magnetic sister compound PdCoO2, indicating that it is a consequence of the coupling to the Mott-insulating layer. Intriguingly, in the region of the T-linear resistivity, the scattering rate per kelvin is well approximated by the ratio of fundamental constants, kB /h. Numerous other materials reveal the same slope in the T-linear region, in spite of large differences in the microscopic origins of the scattering. To investigate the universal behaviour of the scattering rate, we conducted a systematic study of the influence of point defects on the resistivity of PdCrO2, the results of which we report here. We introduced point defects to microstructures of PdCrO2 by irradiating them with high-energy electrons. Comparing the results with those on PdCoO2 , we confirm that the increase in the resistivity is dominated by point defects in conductive Pd layers.

MM 22: Liquid and Amorphous Metals - Metallic Glass

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

MM 22.1 Tue 10:15 IFW D

Effect of Co micro-alloying on thermodynamic and kinetic properties of a $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass — •Rene Hubek, Isabelle Binkowski, Martin Peterlechner, Sergiy Divisinki, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

The physical properties of bulk metallic glasses are subject of intense research especially with respect to their mechanical behavior. Recently, it was shown that the mechanical properties of a $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass could significantly be enhanced through cobalt micro-alloying [1]. In this report, we are focusing on the low-temperature heat capacity and shear band diffusion measurements. The results are discussed in comparison to the reference Co-free Pd40Ni40P20 glass [2, 3]. The response of the excess heat capacity at low temperatures, known as the boson peak, on plastic deformation and post-deformation annealing is thoroughly examined. Furthermore, the influence of annealing and micro-alloying on the shear band diffusion is investigated. These data are discussed with respect to the relaxation behavior. The correlated study of thermodynamic and kinetic properties of deformed glasses provides further insights into origin of plasticity enhancement by Co-micro-alloying of PdNiP-glass.

[1] N. Nollmann et al., Scripta Materialia 111 (2016), 119-122
[2] Y.P. Mitrofanov et al, Acta Materialia 90 (2015) 318-329.
[3] I. Binkowski et al, Acta Materialia 109 (2016) 330-340.

MM 22.2 Tue 10:30 IFW D

Effects of pretreatments on the mechanical properties of metallic glasses — •Hongbo Zhou[1], Yuriy Mitrofanov[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Muenster, Wilhelm-Klemm Strasse 10, Muenster 48149, Germany — [2]Department of General Physics, State Pedagogical University, Lenin Street 86, Voronezh 394043, Russia

Pretreatments including annealing and plastic deformation have a significant influence on the microstructure and non-equilibrium state of metallic glasses such as medium range order and the rejuvenation behavior. Therefore, connecting these influences to the resulting mechanical properties seems very promising to help understanding some basic issues, such as the structural origin of plasticity, heat effects and shear modulus softening. In this work, the samples were pretreated by low-temperature annealing, high-pressure torsion and cold rolling. The energetical state and thermal properties of metallic glasses were evaluated by differential scanning calorimetry and a physical property measurement system. Three-point bending, compression and shear modulus tests were carried out. The relation between mechanical properties and thermal properties was discussed. In addition, the differential scanning calorimetry curve can be reconstructed with the shear modulus data within the framework of the interstitialcy theory, which demonstrates the similar structural origins of the heat effect and shear modulus softening in metallic glasses.

MM 22.3 Tue 10:45 IFW D

Investigation of creep in Pd40Ni40P20 metallic glasses — •Christian Aaron Rigoni, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, Münster, Germany

Metallic glasses are well known for their distinguished mechanical properties like high hardness and tensile strength, but marginal - if any - ductility. Therefore, long-time behaviour of metallic glasses under creep conditions is important for an optimal application of the material in order to prevent unexpected failures. In contrast to crystalline materials, where the creep mechanisms are well understood in terms of evolution of lattice defects, these mechanisms are still not well known for metallic glasses especially at temperatures far below Tg, where plastic deformation occurs through shear banding effecting local areas (shear transformation zones). Pd40Ni40P20 is chosen as a model metallic glass due to its high thermal stability over a wide temperature range and superior glass forming abilities. Even though Pd40Ni40P20 is a good glass former, the casted bulk samples are limited to certain sample dimensions, which makes classical tensile testing machines useless for this application. In our case the measurements are proceeded in a miniaturized tensile testing machine, which uses a sample length of about 4 mm with a gauge section of about 0.3 mm2. The first results on creep behaviour at temperatures 400 to 470 K (more than 100 K below Tg) are presented and discussed.

MM 22.4 Tue 11:00 IFW D

Impact of cryogenic cycling on plastically deformed Pd40 Ni40 P20 bulk metallic glass as studied by tracer diffusion

measurements — •Afrouz Hassanpour, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics University of Münster Wilhelm-Klemm-Str. 10 48149 Münster Germany

Rejuvenation via cryogenic cycling is an intensively investigated, but still obscure phenomenon for bulk metallic glasses. The calorimetric response of cryo-cycled as-cast and relaxation-annealed PdNiP glasses was found to remain practically unchanged. In the present work, tracer diffusion is used as a probe of structural changes induced by cryo-cycling in PdNiP glasses plastically deformed by high-pressure torsion and cold rolling. The penetration profiles for 57Co atoms reveal specific changes when samples were subjected to cryogenic cycling including both volume and short-circuit (shear band) diffusion contributions. The results substantiate a distinct impact of the cryogenic thermocycling on shear transformation zones and shear band structures, with the latter being characterized by significantly enhanced diffusion coefficients. Thus, the shear bands reveal a kind of kinetic rejuvenation induced by cryo-cycling and apparently a higher susceptibilitay for structural modifications through cryo-cycling as compared with undeformed material, at least for the model PdNiP glass.

MM 22.5 Tue 11:15 IFW D

Effect of Gd micro-alloying on thermodynamic, kinetic and mechanical properties of a Pd40Ni40P20 bulk metallic glass — •Saba Khademorezaian[1], Martin Peterlechner[1], Marilena Tomut[2], and Gerhard Wilde[1] — [1]Westfälliche Wilhelms-Universität Münster, Münster, Germany — [2]GSI Helmholtzzentrum für schwerionenforschung, Darmstadt, Germany

In the field of bulk metallic glasses, minor additions have proven to be a powerful tool to enhance different properties, among which glass forming ability, thermal stability and plasticity are forming the focus of this report.

We have studied the impact of adding 1 at% Gd to a reference Pd40Ni40P20 bulk metallic glass on glass forming ability, crystallization kinetics and also fictive glass transition temperature. [1] As Nollmann et al. [2] shown, minor addition of different elements can have a positive or negative impact on the mechanical properties of metallic glasses. The impact of the Gd addition on the glass forming ability was performed by calorimetric analyses and mechanical properties were investigated by compression test as well as by micro- and nanoindentation. Studying the changes in glass plasticity caused by different alloying additions can also provide better knowledge of deformation mechanism, shear band formation and propagation. [3]

[1] Y.P.Mitrofanov et al, Acta Materialia 90 (2015) 318-329 [2] N. Nollmann et al., Scripta Materialia 111 (2016), 119-122 [3] I. Binkowski et al, Acta Materialia 109 (2016) 330-340.

MM 23: Topical Session: Interface-dominated phenomena - Interactions at Interfaces

Time: Tuesday 11:45–13:00 Location: IFW A

MM 23.1 Tue 11:45 IFW A

Elastic Strain Effect in Electrocatalysis during Methanol Oxidation Reaction on Gold/Platinum Thin Films — •Xinyan Wu[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

It is well known that one effective method of enhancing the electrocatalytic performance is to tune the surface strain of nanomaterials, by which the adsorption enthalpies could be modified. However, quantifiable experimental observations of the impact of strain for reactivity of catalyst are still rare, which means this field lacks a quantitative experimental database. Here we explore a method, Dynamic Electro-Chemo-Mechanical analysis (DECMA), in order to investigate the impact of elastic strain on the electrocatalystic methanol oxidation reaction on gold and platinum thin film surface in alkaline solutions. In this way, coupling parameters such as potential-strain & and current-strain Λ coefficients are measured and suggest that tensile strain decreases the adsorption energy thus bring a strong binding between OHads and electrode. However, this stronger binding plays different roles on Au and Pt electrodes, which revealed different strain modulation mechanism in these two systems during methanol oxidation reaction(MOR). Pt electrode responses more strongly and oppositely as Au electrode towards external tensile strain, namely a compressive stain effect is more favourable on Pt electrode.

MM 23.2 Tue 12:00 IFW A

Structure and local electrical resistivity in copper grain boundaries — •Hanna Bishara, Matteo Ghidelli, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung

Grain boundaries (GBs) are among the most significant microstructure defects influencing mechanical and functional properties of materials. The atomic structure at a GB is determined by the crystallography, composition and temperature as well as by the relative orientation between neighbouring grains. Still, the impact of structural characteristics of the GB on the various physical properties of the materials is not fully understood. Here, we aim to correlate the structural and electrical properties of GBs through in-situ local electrical measurements on well-defined GB planes.

To this aim Cu thin films are sputter-deposited and annealed to induce grain growth with final grain sizes of a few tens of micrometers. EBSD is used to identify the GB plane. Subsequently, FIB machining is employed to isolate specific GBs and their corresponding grains from the rest of film, to probe the electrical resistivity. The electrical resistivity measurements are conducted in-situ through 4-point-probe measurements using micro-manipulators and a nV sensitive voltagemeter. We report, for the first time, on direct resistivity measurements of different coincidence site lattice (CSL) and low angle GBs in Cu. Measured resistivities span for more than order of magnitude and match the predicted values by simulations. Deviation from predicted values are related to Ga segregation into GBs. The results provide a solid relation between structure and electrical properties of GBs.

MM 23.3 Tue 12:15 IFW A

Directionality of metal-induced crystallization and layer exchange in amorphous carbon/nickel thin film stacks — •Matthias Krause[1], Daniel Janke[1], Frans Munnik[1], Jaakko Julin[1], René Hübner[1], Jörg Grenzer[1], Christina Wüstefeld[2], David Rafaja[2], and Sibylle Gemming[1,3] — [1]Helmholtz-Zentrum Dresden- Rossendorf, 01328 Dresden, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Straße 5, 09599 Freiberg, Germany — [3]Institute of Physics, TU Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz, Germany

Metal-induced crystallization and layer exchange (LE) of amorphous carbon in thin film stacks with Ni were investigated as a function of the initial stacking order. Bilayer and triple layer stacks were exposed to heating ramps up to 700°C.

Turbostratic carbon formed during annealing. The degree of LE, quantified by ion beam analysis, is 95 % and 80 % for the outward and inward direction, respectively. Based on the calculation of surface and interface energies of the initial and final states, thermodynamic estimations pointed to the wetting of Ni grain boundaries by C atoms as the initial driving force for the LE and allowed a consistent understanding of the LE directionality and of the final thin film microstructure.

MM 23.4 Tue 12:30 IFW A

Atomistic simulation of nucleation during solidification in binary alloys — •Sarath Menon, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität, Bochum

Advances in experimental methods such as fast scanning calorimetry have enabled the study of nucleation during solidification to obtain free energy barriers and reaction rates. Insight into the nucleation mechanism on an atomic scale, however, remains elusive due to the time and length scales of the process. In the case of binary alloy systems, the thermodynamic and kinetic quantities often depend on the concentration, phase separation and phase selection, leading to a complex nucleation mechanism. Here, we employ transition path sampling to calculate thermodynamic and kinetic quantities and to study nucleation mechanisms atomistically. An interesting class of materials are metal-semiconductor compounds. As a model system to approximate such a binary alloy, we use a two-component Stillinger-Weber potential that is able to capture the characteristic features of the phase diagram including the eutectic point. Our results provide information about the concentration dependence of nucleation kinetics and shed light on phase selection and separation during nucleation in binary alloys.

MM 23.5 Tue 12:45 IFW A

Interplay of grain boundaries, deformation and electromagnetic properties in iron silicon steel — •Martin Heller[1], James Gibson[1], Nora Leuning[2], Kay Hameyer[2], and Sandra Korte-Kerzel[1] — [1]Institute of Physical Metallurgy and Material Physics, RWTH Aachen — [2]Institute of Electrical Machines, RWTH Aachen

Iron-silicon electrical steel sheet is the most widely used material for iron cores of electrical machines like generators, motors or transformers. Although already ubiquitous, the demand will nevertheless rise in the future since electro-mobility is spreading rapidly. The magnetic properties of the electrical steel sheet directly influence the application performance. Hysteresis losses result from the movement of domain walls. Even though electrical sheet steel is generally used in a fully recrystallized state, it is the final stages of production involving cutting that introduce large plastic strains, and hence high local dislocation densities. These have been shown to cause significant loss in performance, due to pinning of domain walls by dislocations. This study aims to learn more about the evolving dislocation structures at specific grain boundaries during deformation. Thus, single-crystalline micropillars (2*m x 4*m) are milled in two adjacent grains and their corresponding bi-crystalline counterparts on the grain boundary. After compression mechanical data, slip traces and crystal rotation are further analysed to study the interaction of dislocations on individual slip systems and the grain boundary. In a next step, grain orientations, grain boundaries and evolved dislocation structures will be correlated with electromagnetic properties on the macroscale.

MM 24: Materials for Sensors and Actuators

Time: Tuesday 11:45–13:00 Location: IFW B

MM 24.1 Tue 11:45 IFW B

Supramolecular Functionalized Pristine Graphene Utilizing A Bio-compatible Stabilizer Towards Ultra-sensitive Ammonia Detection — •Shirong Huang[1], Luis Antonio Panes-Ruiz[1], Alexander Croy[1], Leif Riemenschneider[1], Vyacheslav Khavru[2], Viktor Bezugly[1,2,3], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Life Science Inkubator Sachsen GmbH & Co. KG, Tatzberg 47, 01307 Dresden, Germany — [3]Center for Advancing Electronics Dresden (cfAED), TU Dresden, 01062 Dresden, Germany

In this work, we develop pristine graphene-based gas sensors utilizing flavin monocleotide sodium salt (FMNS) towards ultra-sensitive ammonia detection. The sensor has 3% response upon exposure to 10 ppm NH3 and a limit of detection of 1.6 ppm at room temperature and shows a good recovery. Raman, UV-vis, FT-IR spectra, as well as SEM measurements are employed to characterized the quality of the graphene flakes, indicating a good structural quality of graphene with few defects. Complementary molecular dynamics simulation results show that FMNS molecules play two important roles for the graphene sensor: to stabilize graphene flakes via supramolecular functionalization and to act as binding sites for NH3 molecules. The process is very mild, environmentally friendly, and low cost. We believe this work may pave a path to design high performance gas sensor with low cost and boost the application of graphene for sensing.

MM 24.2 Tue 12:00 IFW B

Implantable Highly Compliant Devices for Heating of Internal Organs: Toward Cancer Treatment — •Tetiana Voitsekhivska[1], Gilbert Santiago Canón Bermúdez[1], Tetyana Yevsa[2], Inga Hochnadel[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Department of Gastroenterology, Hepatology and Endocrinology, Hannover Medical School, Carl-Neuberg-Str. 1, 30625 Hannover, Germany

Flexible electronics can revolutionize the health care sector. Despite numerous functional flexible devices already demonstrated, tumor treatment remains unexplored in this field. We realized a highly compliant device for targeted heat treatment of tumor sites of internal organs [1], consisting of a 6 μm-thick polymeric foil hosting a heater and temperature sensor, coated with a 5 μm-thick encapsulation layer. We study the electro-thermal and mechanical characterization of the devices and demonstrate that they can be efficiently used to thermally impact normal and cancerous tissues of autochthonous murine models with liver cancer. The device withstood more than 50 bending cycles at 2.5 mm bending radius, retaining the accuracy of 0.2 °C. The developed highly compliant device paves the way for handling of exophytic tumor nodules via thermal destruction of tissue, targeted drug release, or enhancement of antitumor immune responses.

[1] G.S. Canón Bermúdez et al., Adv. Eng. Mater. 21, 1900407 (2019).

MM 24.3 Tue 12:15 IFW B

High compliancy for printed magnetic field sensors — •Minjeong Ha[1], Gilbert Santiago Cañón Bermúdez[1], Tobias Kosub[1], Yevhen Zabila[2], Rico Illing[1], Yakun Wang[1], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]The H. Niewodniczanski Institute of Nuclear Physics, Krakow, Poland

The development of highly-compliant and skin-conformal magnetic sensors is essential for the human-interactive electronics capable of position recognition and tracking motion. To design such human interactive sensing devices, printing technique is a great approach due to easily tunable and shapable process, cost-effectiveness, and large-area fabrication. Here we report printable magnetoresistive sensors on ultra-thin films that can naturally comply with the skin. Thanks to the new formulation of the paste, the printed magnetic microflakes could firmly attach to any even ultrathin polymeric substrate showing mechanical stability under 16 um bending radius without any damage. The excellent percolation contacts between the randomly distributed microflakes attribute the high sensitivity of 2.2/T in low magnetic field ranges of 1 mT on the bending curvature of 500 um, resulting in 1900 times higher figure of merits than current state-of-the-art printable magnetic sensors. With this performance, our printed sensors on skin demonstrate a touchless control of virtual objects for the practical application in human-interactive wearable devices, artificial prosthetics, robotics, and internet of things.

MM 24.4 Tue 12:30 IFW B

Generation of core-gap-shell microcapsules for stimuli-responsive biomolecular sensing. — •Hyejeong Kim[1], Seong min Jo[2], Fanlong Meng[1], Yinzhou Guo[2], Héloïse thérien Aubin[2], Ramin Golestanian[1], Katharina Landfester[2], and Eberhard Bodenschatz[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Stimuli-responsive microparticles carrying dedicated cargo have great potential in a variety of technical applications, such as sensor and actuator technologies, drug delivery and catalysis. Here we report results on thermo-responsive core-gap-shell microcapsules (TCGSM) made of Poly(N-isopropylacrylamide), which allow the encapsulation of hydrophilic payloads in a simple, stable, and reliable manner. Different designs of TCGSM were realized by individually controlling the swelling of the inner core and the outer shell or by incorporating pH-responsive co-monomers into the inner core. The gap, i.e. the space between the inner core and the outer shell, can be loaded with dedicated cargo such as nanoparticles. The outer shell can serve as a stimuli-responsive gateway for the exchange of smaller molecules with the external aqueous solution. This is demonstrated with the realization of a temperature controllable enzymatic glucose sensor. The presented platform opens new avenues for the production of stimuli-responsive core-gap-shell microparticles for a multitude of applications.

MM 24.5 Tue 12:45 IFW B

Fabrication of ZnO/Si NWs p-n Heterojunction array based High Response Nitric Oxide (NO) Gas Sensor with Noise Limited Detectivity Approaching 10 ppb — •Chandan

Samanta, Ankita Ghatak, A K Raychaudhuri, and Barnali Ghosh — S N Bose National Centre for Basic Sciences, Kolkata, India

Gas sensors, particularly those based on solid state devices are commercially available and are widely used to hazardous gas monitoring and new vistas for application are opening up for solid state gas sensors for use in healthcare such as exhaled breath analysis. In this work we report a ZnO/Silicon nanowires (ZnO/Si NWs) based p-n heterojunction diode array based Nitric Oxide (NO) gas sensor that can show a calibrated detection capability at least down to 0.5ppm (with dry N2 as the ambience gas). Utilization of cost effective chemical technique for fabrication of sensor on silicon is compatible with wafer level processing and easily connecting with silicon IC technology. The vertically aligned Si NWs array has been made by electroless etching method and the ZnO nanostructure was made by chemical solution deposition and spin-coating. We observe that the heterostructure leads to a synergetic effect where the sensing response is more than the sum total of the individual components. Extensive cross-sectional electron microscopy and composition analysis by line EDS allowed us to make a physical model. The comparison of the simulation results with the experiment point out the device parameters that enhance the device response.

MM 25: Liquid and Amorphous Metals - Structure

Time: Tuesday 11:45–13:00 Location: IFW D

MM 25.1 Tue 11:45 IFW D

TEM in-situ investigation of local dynamics in amorphous alloys — •Katharina Spangenberg, Sven Hilke, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

The investigation of the amorphous atomic structure in metallic glasses (MGs) is essential for production and design of MGs as engineering materials. Unlike crystals, MGs have no long-range order, but may consist of distinct atomic structures often summarized as medium-range order (MRO). The degree and type of MRO in amorphous materials can be measured by fluctuation electron microscopy (FEM) using the evaluation of spatial fluctuations in diffraction from nanoscale volumes or intensity variations in dark field images. It has been experimentally shown that the dynamics of MGs in terms of atomic mobility are related to their mechanical properties and connect to the underlying mechanisms of plastic deformation. Therefore, spatial maps of atomic fluctuations can be evaluated to give insight into typical time and length scales of these rearrangements. In this sense, electron correlation microscopy (ECM) is able to investigate dynamics and relaxation phenomena at the atomic scale. The focus of the presented study is the atomic structure of nanostructured MGs using the techniques of ECM in TEM. The dynamics of nanostructured MGs are analysed at different temperatures. Different sample preparation routes are presented and the possibilities of in-situ sample analysis, which enables an observation of the microstructure and reactions at the atomic level upon e.g. heat or mechanical treatment, are discussed.

MM 25.2 Tue 12:00 IFW D

Uncovering β-relaxations in amorphous phase-change materials — •Shuai Wei[1], Si-xu Peng[2], Yudong Cheng[1], Julian Pries[1], Hai-bin Yu[2], and Matthias Wuttig[1] — [1]RWTH Aachen University — [2]Huazhong University of Science and Technology

Relaxation processes are decisive for many relevant physical properties of amorphous materials. For amorphous phase-change materials (PCMs) employed in non-volatile memories, relaxation processes are, however, difficult to characterize due to the lack of bulk samples. Here, instead of bulk samples, we use powder mechanical spectroscopy for powder samples to detect the prominent excess wings– a characteristic feature of β-relaxations – in a series of amorphous PCMs at temperatures below the glass transition. By contrast, β-relaxations are vanishingly small in amorphous chalcogenides of similar composition, which lack the characteristic features of phase-change materials. This conclusion is corroborated upon crossing the border from PCMs to non-PCMs, where β-relaxations drop significantly. Such a distinction implies that amorphous PCMs belong to a special kind of covalent glasses whose locally fast atomic motions are preserved even below the glass transitions. These findings also suggest a correlation between β-relaxation and crystallization kinetics of PCMs, which may have technological implications for phase-change memory functionalities.

MM 25.3 Tue 12:15 IFW D

Controlling the Effective Cooling Rate upon Magnetron Sputter Deposition of Glassy Ge15Te85 — •Julian Pries[1], Shuai Wei[1], Felix Hoff[1], Pierre Lucas[2], and Matthias Wuttig[1,3] — [1]Institute of Physiks IA, RWTH Aachen — [2]Department of Material Science and Engineering, University of Arizona — [3]PGI-10, Forschungszentrum Jülich

A reduction of the enthalpy state is accompanied by a desirable stabilization of the glass. In this study, we demonstrate the relationship between the voltage applied in the sputtering process and the resulting enthalpy state. Due to this correspondence, it is possible to assign an effective cooling rate to the sputtering process, which decreases by about three orders of magnitude when the voltage is increased by ~100 V. This shows that the sputtering voltage as a new and decisive parameter can manipulate the fictive temperature of a glass, which opens the door to the design of ultra-stable, but also ultra-unstable glasses.

MM 25.4 Tue 12:30 IFW D

Correlating transmission electron microscopy data to study dynamics in amorphous structures — •Martin Peterlechner, Sven Hilke, Katharina Spangenberg, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster

The method of transmission electron microscopy (TEM) is well suited to study atomistic structures and their dynamics. However, due to the quantum-mechanical interference of electrons with matter, the arising contrast is not straight forward to interpret. Moreover, any quant can alter the observed object, generally termed beam damage in the TEM community. Thus, either correlations of image simulations with individual experimental micrographs are used, or, more recently time autocorrelations of signals obtained by TEM. In the present work, the choice of signals for time correlations is elucidated and experimental limitations are discussed. To link the experiments to physical quantities the relaxation of an amorphous structure is analysed.

MM 25.5 Tue 12:45 IFW D

Pure Néel-type Spin Textures in Ferrimagnetic Alloys — •Boris Seng[1,2,3,4], Daniel Schönke[1], Nico Kerber[1,3,4], Fabian Kammerbauer[1], Jean-Loïs Bello[2], Daniel Lacour[2], Robert Reeve[1], Michel Hehn[2], Stéphane Mangin[2], and Mathias Kläui[1,3,4] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Institut Jean Lamour, 2 allée André Guinier, 54011 Nancy Cedex, France — [3]Max Planck Graduate Center, Staudingerweg 9, 55128 Mainz, Gemany — [4]Graduate School of Excellence Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany

Magnetic skyrmions are topologically stabilized spin textures that have been suggested for next generation spintronics devices. Recent studies confirmed the current-driven skyrmion dynamics in ultrathin ferromagnets. However, the Magnus effect leads to a transverse motion of ferromagnetic skyrmions for spin structures with a non-zero topological winding number. Antiferromagnetically exchange-coupled skyrmions or compensated ferrimagnets are expected to suppress this effect owing to an overall zero topological charge. Especially at the angular momentum compensation temperature skyrmions dynamics is predicted to be collinear with the current[1]. Here, we explore GdFeCo ferrimagnetic alloy-based multilayer stacks where a strong Dzyaloshinskii-Moriya interaction is present. In our samples, we observe chiral spin textures such as magnetic skyrmions. The spin distribution of their internal domain walls is imaged and found to be a pure Néel-type.

[1] Barker et al., Phys. Rev. Lett. 116, 147203 (2016)

MM 26: Topical Session: Data Driven Materials Science - Machine Learning for Materials Properties

Time: Tuesday 14:15–15:30 Location: BAR 205

MM 26.1 Tue 14:15 BAR 205

From Atom Probe Tomography to CALPHAD modeling: Estimating T_c from local concentration fluctuations — •Marvin Poul, Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Germany

One way to determine the extent of the miscibility gap and the associated critical solution temperature T_c in binary alloys from Atom Probe Tomography (APT) is to prepare nano-layer stacks, anneal them and determine the respective layer concentrations, which mark the boundaries in the phase diagram. Since this relies on diffusion, it can be problematic when T_c and atomic mobilities are low, such as in Cu/Ni, leading to long annealing times.

This work proposes a novel methodology based on statistical mechanics to extract T_c from histograms of thermodynamically inherent local concentration fluctuations annealed above T_c, i.e. in the region of complete miscibility. The same formalism allows to extract relative chemical potential differences from two or more samples with different mean concentration. Given enough data to span the full concentration range it is even possible to non-parametrically recover the excess free energy of mixing $g_{ex}(c)$, which allows a direct approach to a CALPHAD parametrization.

The approach is benchmarked using Embedded Atom Monte Carlo simulations of Cu/Ni and applicability to experimental histograms from APT is discussed.

MM 26.2 Tue 14:30 BAR 205

Analysis of magnetic properties in the Fe-Si system using first principles calculations — •Matteo Rinaldi, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

Magnetic steels containing small amounts of silicon have been used extensively as soft magnetic materials in various technological applications. The behavior of magnetic materials can be simulated at the macroscale using a micromagnetic model whose key parameters, such as exchange stiffness constants and magnetic anisotropies can be derived from first-principles electronic structure calculations. In our work, we employ Korringa-Kohn-Rostoker (KKR) Green's function calculations together with a Wannier-based tight-binding (TB) method to investigate the dependence of the spin-wave stiffness and the first coefficient of the cubic magneto-crystalline anisotropy on the Si concentration. These two methodologies give a chemical and structural description of the changes in the micromagnetic parameters caused by the addition of Si. The KKR method is used in conjunction with the Coherent Potential Approximation to simulate chemical disorder while the TB method addresses local relaxations induced by the presence of Si in a supercell framework. The role played by the hybridization between the Si and Fe orbitals turned out be decisive to explain the trends in the micromagnetic parameters. Our calculated values are in excellent agreement with available experimental data.

MM 26.3 Tue 14:45 BAR 205

Machine learning modeling of magnetic ground state and Curie temperature — •Teng Long, Nuno Fortunato, Yixuan Zhang, Oliver Gutfleisch, and Hongbin Zhang — Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany

Magnetic materials have a plethora of applications ranging from information and communication technologies to energy harvesting and conversion. However, their functionalities are often limited by the magnetic ordering temperature. In this work, we performed machine learning on the magnetic ground state and the Curie temperature (T_c), with generic chemical and crystal structural descriptors. Using 2805 known intermetallic compounds, a random forest model is trained to classify ferromagnetic and antiferromagnetic compounds and to predict the T_c of the ferromagnets, with only 15 and 23 descriptors used, respectively. The resulting accuracy is about 86% for classification and 92% for regression (with a mean absolute error (MAE) of 55K). We found that composition based features are sufficient for both classification and regression, whereas structural descriptors improve the performance. Using the trained model, we predicted the magnetic ordering and T_c for the intermetallic magnetic materials in the Materials Project, with a MAE of 73K in comparison to the experimental reported T_c that has been collected by us. This work paves the way to accelerate the discovery of new ferromagnetic compounds for technological applications.

MM 26.4 Tue 15:00 BAR 205

Automatization of magnetic properties calculation using AiiDA-FLEUR — •Vasily Tseplyaev, Jens Bröder, Daniel Wortmann, Markus Hoffmann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic properties of thin films, e.g. magnetic anisotropy, Heisenberg exchange and Dzyaloshinskii-Moriya interaction constants define material quality for possible use in state-of-the art memory and other devices. These parameters can be determined via *ab initio* theory and the FLEUR [1] code. Together they provide precise simulations with the necessary predictive power. The current state of computational resources allows for high-throughput screening of materials, which means similar calculations are repeated for a large set of possible magnetic film structures that can be promising for further experimental study. Automated computing, data storage, provenance and thus reproducibility are provided by the open science platform AiiDA [2], when key-turn solutions for aforementioned magnetic calculations are implemented as AiiDA-FLEUR plugin. In this talk, we report the current state of AiiDA-FLEUR development, which covers the implemented architecture of general and magnetic workflows and other utilities.

We acknowledge the Center of Excellence MaX – Materials Science at the Exascale (EU H2020-INFRAEDI-2018) for financial support.

1. https://www.flapw.de
2. G. Pizzi *et al.*, Comp. Mat. Sci. **111**, 218 (2016).

MM 26.5 Tue 15:15 BAR 205

Screening impurity effects in topological insulators with the AiiDA-KKR plugin — •Philipp Rüssmann[1], Fabian Bertoldo[1,2], Phivos Mavropoulos[3], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Technical University of Denmark, Kgs. Lyngby, Denmark — [3]Physics Department, National and Kapodistrian University of Athens, Greece

The ability to utilize the predictive power of *ab initio* calculations through automated computing enables scanning of the material space with subsequent materials/properties optimization. We present the *AiiDA-KKR* plugin [1] which enables high-throughput calculations using the Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method (KKR) [2] to the AiiDA framework [3]. The KKR method allows, for instance, to calculate the electronic structure of defects embedded into crystalline solids. We applied this scheme to screen the effect of impurities in the strong topological insulator Sb_2Te_3. Several thousand impurities have been considered, taking into account both the distance of the impurity to the surface as well as the effect of possible changes in the host material's Fermi level. Our data reveals chemical trends relevant, for example, to transport properties in topological insulators. – We acknowledge the Center of Excellence MaX (EU H2020-INFRAEDI-2018) for financial support.

[1] https://github.com/JuDFTteam/aiida-kkr
[2] https://jukkr.fz-juelich.de
[3] G. Pizzi, *et al.*, Comp. Mat. Sci. **111**, 218-230 (2016).

MM 27: Topical Session: Interface-dominated phenomena - Nanoporous Metals

Time: Tuesday 14:15–15:30 Location: IFW A

MM 27.1 Tue 14:15 IFW A

Precipitation in nanoporous Au-Ni — •Maowen Liu[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

The vacancies formed during dealloying process play a critical role in the preparation of nanoporous metals. In order to obtain a detailed understanding of the vacancy distribution in nanoporous metals, the precipitation behavior, which can reflect the vacancy migration and is closely related to the void distribution, was investigated. In the present work, Au-Ni alloy, a typical immiscible binary alloy, was selected for the study of precipitation. The precipitation behavior in nanoporous Au-Ni during dealloying and subsequent heat treatment was investigated using a transmission electron microscopy equipped with an energy dispersive X-ray spectroscopy. The results reveal that parts of Ni atoms tend to aggregate as nanoscale clusters in the nanoporous alloy during dealloying process. After heat treatment, more Ni precipitates appear in the ligaments. It is speculated that the Ni clusters and some small voids formed during dealloying process provide nuclei for the subsequent precipitates.

MM 27.2 Tue 14:30 IFW A

Hybrid Materials Made from Nanoporous Metals and Electrically Conductive Polymers as Electro-Chemo-Mechanical Actuators — •Benedikt Roschning[1] and Weissmüller Jörg[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

Nanoporous metals can be used as functional materials like sensors or actuators, due to their high intrinsic, externally accessible surface. The mechanism is based on surface stress variations as a consequence of an applied electrical potential. This stress variation acts on the underlying bulk atoms, resulting in actuation, scaling with the feature size. The environmental stability and structural coarsening due to surface diffusion restricts the materials choice to noble metals like gold or platinum and are still an issue in terms of long-term stability. Another class of electro-chemo-mechanical actuators are conductive polymers. Their actuation is caused by the incorporation of co-ions between the polymer chains for charge balancing. Within thin films, fast ion exchange is possible, but the stiffness of the underlying substrate limits the effect of actuation. A combination of both approaches, the coating of the intrinsic surface area of nanoporous metals with electrically conductive polymers, leads to superior electrochemical and actuatoric properties. Within this contribution, we address manufacturing approaches, the electrochemical properties as well as the underlying mechanisms for actuation.

MM 27.3 Tue 14:45 IFW A

Coarsening of nanoscale metal networks and their connectivity evolution via kinetic Monte Carlo simulations — •Yong Li[1,2], Bao-Nam Dinh Ngo[2], Jürgen Markmann[2,1], 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

Nanoporous gold made by dealloying takes the form of a network assembled from nanoscale struts or "ligaments". It has been emphasized that the connectivity of the networks is decisive for their mechanical behavior. The relevant experimental observations lead to apparently contradictory conclusions on how the connectivity evolves during coarsening. Here, we study the microstructure evolution of nanoscale metal network structures due to surface diffusion during annealing, using large-scale on-lattice kinetic Monte Carlo simulation and spinodal-like initial microstructures. Our results [Y. Li et al., Phys Rev Mater 3 (2019) 076001.] confirm the classical time exponent $t^{1/4}$ for the size evolution. They also reveal that the degree of surface faceting does not affect the growth kinetics or the evolution of connectivity. The initial connectivity, as described by a scaled topological genus, depends on the solid fraction, φ, of the microstructure. Furthermore, networks with $\varphi \geqslant 0.30$ undergo a self-similar coarsening and maintain their connectivity, whereas networks with $\varphi < 0.30$ lose their connectivity during coarsening and will eventually disintegrate into isolated clusters.

MM 27.4 Tue 15:00 IFW A

Electrochemically driven actuation and change in Young's modulus of nanoporous metal-conductive polymer actuator under external load — •Jie Li[1], Jürgen Markmann[1,2], Jörg Weissmüller[1,2], and Nadiia Mameka[1] — [1]Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics — [2]Hamburg University of Technology, Institute of Materials Physics and Technology

Nanoporous (np-) metals made by dealloying may be considered as promising low-voltage electro- and chemo-mechanical actuators with a good combination of actuation strain, stiffness and strength [1]. The actuation performance of np metals can be further improved by electrodeposition of conductive polymers on the pore surface [2]. Here, we study hybrid electroactuator from np Au and polypyrrole (PPy). Upon electric charging in an aqueous electrolyte, the material exhibits actuation as well as large modulation in stiffness. We point out that the stiffness change can strongly affect the actuation efficiency-as described by the maximum work density-particularly when the actuator operates under external mechanical load [3]. We employ a dynamic mechanical analysis with an electrochemical control to study the impact of the applied load on the actuation and the Young's modulus variation. The conditions under which the np Au/PPy actuator shows enlarged actuation amplitudes along with enhanced elastic response will be discussed. [1] L.-H. Shao et al., *RSC Nanoscience-Nanotechnology* 2012, **22**, 137. [2] K. Wang et al, *Sens Actuator B Chem*, 2017, **248**, 622. [3] L.-Z. Liu et al, *Phys Rev Mat*, 2019, **3**, 066001.

MM 27.5 Tue 15:15 IFW A

Nanoporous gold with controlled surface morphology — •Stefan Berger[1], Lingzhi Liu[1,2], Jürgen Markmann[3,1], and Jörg Weissmüller[1,3] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht — [2]Chinese Academy of Sciences, Institute of Metal Research, Shenyang National Laboratory for Materials Science — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg

Nanoporous gold is a nanostructured material with a high specific surface area. The large surface of the nano sized gold structures make the material interesting for applications like catalysis and sensing. Investigations of the catalytic behaviour of gold have shown surface dynamics and surface reconstructions. Based on these findings, we present a method to control the surface morphology by annealing in different gaseous environments. Surface morphology investigations by electron microscopy are presented to classify different faceting behaviour. We show that oxygen is a strong driver for faceting and that high index surfaces appear on gold nano ligaments, when treated in oxygen containing environments. A Oxygen free reducing environment in carbon monoxide in contrast will produce more roughed surfaces with only low index facets. A controlled surface morphology might help to further tune the surface properties, which have a great impact on the bulk properties of nanoporous materials.

MM 28: Computational Materials Modelling - Hydrogen in metals

Time: Tuesday 14:15–15:15 Location: IFW B

MM 28.1 Tue 14:15 IFW B

Understanding rate dependent hydrogen embrittlement in polycrystalline nickel — •Ali Tehranchi, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Hydrogen embrittlement (HE) is a persistent mode of failure in metals. It is well known that hydrogen decreases the fracture energy of grain boundaries (GBs) and promotes intergranular fracture. Hydrogen also increases the critical stress for dislocation-GB reactions. As a consequence, more populated pile-ups of the dislocations will form near the GBs. The dislocations in these pile-ups can attract more hydrogen atoms due to their stress field and deliver them to the GB and facilitate the formation of intergranular crack nuclei. If the length of the crack nucleus is larger than a certain critical length it can propagate along the GB without any need for long-range diffusion of H atoms from the bulk, causing embrittlement. In this work, atomistic simulations of the dislocation-GB interactions are used to demonstrate the increase in the critical stress. The energetics and kinetics of the population of the hydrogen atoms around the dislocation pile-up are presented and discussed. A criterion for fast intergranular fracture is given. This criterion explains the rate dependent experimental observations of HE in nickel as a representative fcc metal. The proposed framework is general and can be used for the prediction of HE in other metallic polycrystals.

MM 28.2 Tue 14:30 IFW B

Hydrogen-Metal Surface Interactions Under Strong Electric Fields — •Michael Ashton, Christoph Freysoldt, and Jörg Neugebauer — Max Planck Institut für Eisenforschung, Düsseldorf, Deutschland

The way that hydrogen arrives at and interacts with charged metal surfaces has important implications for catalysis, corrosion, field evaporation, and energy storage. With a focus on the most ubiquitous hydrogen sources (atomic H, H2, and H2O) interacting with prototypical metal surfaces under strong (~10 V/nm) fields, we use ab initio calculations to investigate energetic pathways for forming some simple hydride molecules that have been observed during field evaporation of tungsten and magnesium. Our results shed light on the fundamental behavior of hydrogen under extreme fields, providing particular insight into the origin and role of hydrogen in atom probe tomography experiments where it is *unintentionally* detected from the environment.

MM 28.3 Tue 14:45 IFW B

A grand canonical approach for modelling hydrogen trapping at vacancies in α-Fe — •Michael W. Finnis[1], Erlend R. M. Davidson[1], Thomas Daff[2], and Gábor Csanyi[2] — [1]Thomas Young Centre, Imperial College London, UK — [2]Engineering Laboratory, University of Cambridge, UK

Vacancies in iron are a potential trap for hydrogen, of importance in the understanding of hydrogen embrittlement of steel. We present a grand canonical approach to computing the trap occupancy, which deals with the entire range of hydrogen concentration, from practically zero to super-saturation. Our method is demonstrated here for hydrogen in α-Fe as a function of both temperature and bulk concentration, using a machine-learned H-Fe potential that we develop for the purpose, which enables rapid sampling with near density-functional theory accuracy. The statistical mechanical calculation of the trap occupancy is enabled by the technique of nested sampling. The almost universally used conventional assumption based on Oriani theory is that at industrially relevant concentrations and ambient conditions vacancy traps are fully occupied. In contrast we find that vacancy traps are less than fully occupied under these conditions, necessitating a reevaluation of how we think about *mobile hydrogen* in iron and steel.

MM 28.4 Tue 15:00 IFW B

Atomistic simulations of hydrogen interactions with dislocations in bcc Fe — •Tapaswani Pradhan, Daria Smirnova, Sergei Starikov, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

The presence of hydrogen degrades the mechanical properties of many metallic materials - the phenomenon known as hydrogen embrittlement (HE). One of the possible reasons of HE is the interaction of H with dislocations that leads to changes in dislocation cores and hence affects their intrinsic glide behavior. Atomic scale details of these interactions and especially the interplay between hydrogen diffusion and dislocation motion is still not fully understood. In this work, we investigate the interaction of H with three types of dislocations, namely, edge, mixed and screw, in body-centred cubic Fe using atomistic simulations. The simulations were carried out using two interatomic interaction models, a tight-binding-based magnetic bond order potential (BOP) and an empirical angularly dependent potential (ADP). Our study shows that H prefers to segregate to all dislocation cores but impacts more the mobility of the glissile mixed and edge dislocations whose Peierls barriers are very low. We present a detailed comparison of simulation predictions and discuss their relation to the HE phenomenon.

MM 29: Materials for Energy Storage and Conversion - Battery and Fuel Cell Materials (joint session MM/CPP)

Time: Tuesday 14:15–15:45 Location: IFW D

MM 29.1 Tue 14:15 IFW D

Atomistic simulation of working interfaces: Towards understanding the role of complex multiphase grain boundaries in all-solid-state Li-ion batteries — •Sina Stegmaier[1], Roland Schierholz[2], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Theoretische Chemie, TU München — [2]IEK-9, Forschungszentrum Jülich

All-solid-state batteries (ASSBs) present a next-generation technology, promising increased operation safety and lifetime as compared to state-of-the-art Li-ion cells. The performance of solid-state electrolytes (SSEs) in ASSBs, though, is severely limited by poorly understood interfacial processes. Atomistic insight into the structure and transport processes at working SSE grain boundaries (GBs) [1] is required to enable rational progress.

To this end, we employ molecular dynamics (MD) simulations with a first-principles parametrized force field and study complex multiphase GBs in the SSE material LATP. An experimentally guided sinter protocol is established to model the formation of semi-amorphous domains at the interface of crystalline LATP grains. The resulting structural atomistic models enable the investigation of anisotropic lateral and transverse ion transport and the comparison to macroscopically accessible observables such as ion conductivity. Following this approach, we leverage experimental input for computational modeling and studying of more realistic solid-solid working interfaces.

[1] A. Mertens et al., Solid State Ionics 309, 180 (2017).

MM 29.2 Tue 14:30 IFW D

Polaron Hopping Mechanism as a source for electronic conductivity in $Li_4Ti_5O_{12}$ (LTO) Batteries — •Matthias Kick[1], Cristina Grosu[1,2], Markus Schuderer[1], Christoph Scheurer[1], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Forschungszentrum Jülich

State of the art lithium ion batteries rely on graphite as anode material due its remarkable lithium-intercalation properties. However due to the low intercalation potential of graphite, Li dendrite growth can occur during rapid charge processes, rendering a potential risk of having short-circuits in a battery cell. In addition, the large volume change during (dis)charging the battery results in unfavorable strain damaging the anode. Lithium titanium oxide $Li_4Ti_5O_{12}$ (LTO) shows the potential of being an excellent alternative to graphite anodes, as its volume stays stable during charge cycles and its high intercalation potential prevents Li dendrites to form. Unfortunately, the low conductivity of LTO still limits its use. To improve on this drawback, an elegant way is to introduce oxygen vacancies resulting in formation of Ti^{3+} centers. As a result, this blue colored LTO shows a lowering in its electronic resistance with improved electronic conductivity. By performing *Hubbard corrected density functional theory* (DFT+U) calculations we are able to show that in fact polaron formation and a possible polaron hopping mechanism can play a significant role in the experimental observed improved conductivities. Morevover we are able to gauge polaronic charge mobility by explicitly calculating polaron hopping barriers.

MM 29.3 Tue 14:45 IFW D

Exploring defect structures in $Li_4Ti_5O_{12}$ (LTO): A combined theoretical and experimental approach — •Yute Chan[1], Cristina Grosu[1,2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]TU München — [2]IEK-9, FZ Jülich

Spinel $Li_4Ti_5O_{12}$ (LTO) is a fascinating anode material for next-generation all-solid-state Li-ion batteries (ASSB). Its "zero strain" charge/discharge behavior promises high safety and long cycling lifetimes. Nonetheless, pristine, white LTO possesses poor ionic and electronic conductivity. The latter can be increased by tailoring the sintering protocol to produce oxygen vacancies, resulting in a performant, blue LTO material. Heretofore, the detailed structure and distribution of the vacancies are unknown. Thus, powerful analytic techniques are needed to identify the defect structure inside the material. Positron lifetime spectroscopy (PALS) stands out from other experimental methods by the ability to sensitively collect positron lifetimes that correlate to different material defects. Data measured at the Garching positron source indicates that the positron lifetimes for LTO bulk and surface are distinguishable. To invert these lifetimes and gain information for the respective regions, we construct a series of LTO bulk and slab models and calculate theoretical lifetimes using two different self-consistent schemes within the framework of two-component density functional theory. We will discuss the relationship between experimental and theoretical lifetimes of LTO bulk and surface.

MM 29.4 Tue 15:00 IFW D

A Neural Network Potential for Lithium Manganese Oxides — •Marco Eckhoff[1], Peter E. Blöchl[2], and Jörg Behler[1] — [1]Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany — [2]Technische Universität Clausthal, Institut für Theoretische Physik, Leibnizstraße 10, 38678 Clausthal-Zellerfeld, Germany

The lithium manganese oxide spinel $Li_xMn_2O_4$, with $0 < x < 2$, is an important cathode material in lithium ion batteries. The recently introduced local hybrid density functional PBE0r yields an accurate description of this material in good agreement with experiment. However, the accessible system size of molecular dynamics and Monte Carlo simulations is very limited when using density functional theory directly. Building on PBE0r data, we thus constructed a high-dimensional neural network potential, which provides a first-principles quality description of the potential energy surface at a fraction of the computational costs. This potential enables large-scale simulations of $Li_xMn_2O_4$ to study phase transitions and lithium diffusion.

MM 29.5 Tue 15:15 IFW D

One parabola to fit them all: A response surface approach to computational catalyst screening — •Frederic Felsen, Christoph Scheurer, and Karsten Reuter — TUM, Munich, Germany

In the pursuit of sustainable power-to-fuel (P2X) technologies methanol fuel from renewable resources is one promising route towards reducing global carbon dioxide emissions. One of the many obstacles to overcome on the way to this ambitious goal is the efficient conversion of CO_2 rich syngas to methanol. Intricate interface structures are characteristic for all commonly employed catalyst materials for this process, like the state of the art $CuZnOAl_2O_3$ [1]. Understanding these surface effects is key for a rational improvement and design of future catalysts.

We present an approach to efficiently characterize solid-solid interface structures by a well defined set of single point DFT calculations. Exploiting ideas from response surface methodology [2], we actively distort interface structures to evaluate the response of the system on geometric changes. Resulting observables such as adsorption energies of reaction intermediates may directly provide insight into the catalytic activity of the respective interfaces. Furthermore, this novel interface characterization may enable computational screening for multi component catalyst materials. As a first test case metal thin films supported on transition metal oxides will be studied.

[1] M. Behrens et al., *Science*, 336, (2012).

[2] R. H. Myers et al., Response Surface Methodology, *Wiley*, (2009).

MM 29.6 Tue 15:30 IFW D

Analysis of $Li_xMn_2O_4$ for catalysis of the oxygen-evolution-reaction (OER) using STEM-EELS — •Florian Schönewald[1], Max Baumung[1], Marcel Risch[1,2], and Cynthia Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Helmholtz-Zentrum Berlin für Materialien und Energie

Controlling the OER is an important step for achieving a sustainable renewable energy future. The process of generating molecular oxygen from water by chemical means is severely kinetically limited. Here $Li_xMn_2O_4$ is studied as a model electrocatalyst. To understand the role of manganese valence and covalency for the OER these are manipulated by electrochemical de-/lithiation. Characterisation of the particles is performed before and after OER, for different lithiation states. Specific attention is given to Mn at the surface since it is directly involved in electron transfer.

With EELS of the O K- and Mn L-edge a surface layer with strongly reduced Mn has been discovered and attributed to changes in Mn/O ratio. This state is also preserved under delithiation. In previous studies, this effect has been explained by tetragonal Mn_3O_4 forming at the surfaces [1]. However, no second phase matching Mn_3O_4 or related structures was identified by X-ray powder diffraction. According to the estimated surface volume share of about 10 %, Mn_3O_4 formation can be excluded. Instead, a combination of oxygen vacancies and additional manganese on tetrahedral sites as antisite defects is taken into account to explain the apparent Mn valence change at surfaces.

[1] Daichun Tang et al, Chem. Mater. 2014, 26, 11, 3535-3543

MM 30: Poster Session II

Time: Tuesday 18:15–20:00 Location: P4

MM 30.1 Tue 18:15 P4

The interplay of geometry and chemistry at Al grain boundaries: insight from atomistics — Liam Huber, •Poulami Chakraborty, Huan Zhao, Baptiste Gault, Dierk Raabe, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Metallic microstructures evolve towards configurations which minimize their free energy. At the mesoscopic scale this involves the coarsening of the polycrystalline grain structure to minimize interfacial energy, but at a finer scale this interface energy can also be reduced through the formation of facets and by solute segregation. Experimental evidence from an Al-Zn-Mg-Cu alloy shows faceting of grain boundaries in this system, and a strong correlation between the grain boundary facet (i.e. geometry) and local chemistry. Using atomistic simulations, we investigate the underlying nano-scale interactions which lead to these facet-specific behaviours. A special focus is placed on the relationship between GB segregation states, which we call ‘defect phases’ when they are thermodynamically (meta)stable, and precipitate structure to give insight into precipitate formation in this system.

MM 30.2 Tue 18:15 P4

Resolving the grain boundary structure in nanocrystalline titanium thin films — •Vivek Devulapalli, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Titanium (Ti) is an important engineering material owing to its high strength-to-weight ratio and biocompatibility. Nanocrystalline Ti (nc-Ti) can have many engineering applications making it necessary to understand the role of interfaces on material properties. However, direct atomic scale observations of GB structures in Ti are lacking and are revealed in this study using aberration corrected scanning transmission electron microscopy (STEM). In a first step, the microstructure evolution of Ti thin films obtained by different deposited techniques was investigated. Substrate temperature, ion flux and growth rate were varied to obtain textured thin films with defined tilt grain boundaries. The global film microstructure, which varied from single crystalline to nano-crystalline with different degrees of texture, were then investigated using XRD, SEM and EBSD. A nc-Ti film deposited on Si (100) contained a myriad of low angle grain boundaries and showed strong [0001] fibre texture. The atomic structure of these boundaries was further investigated by STEM. A grain boundary with 13 deg misorientation and [0001] tilt axis was composed of a dense network of [11-20] edge dislocations with a uniform spacing of 1.3nm. The intrinsic details of film growth and the resulting grain boundary structures will be discussed.

MM 30.3 Tue 18:15 P4

Observing the atomic structure of [111] tilt grain boundaries in Al — •Saba Ahmad, Christian Liebscher, and Gerhard Dehm — Max-Planck-Institute for Iron Research, 40237 Düsseldorf, Germany

Grain boundaries can be described as interface-stabilized phases which exhibit transitions between different states. These transitions are marked by discontinuous changes in grain boundary properties like mobility, cohesive strength and sliding resistance, etc. that are governed by the structure and chemistry of a grain boundary. Understanding the atomic structure of these interfacial states and the way it influences the GB properties can pave the way for GB engineering. But, a detailed understanding of the atomic structure of the GBs and their atomistic segregation behaviour is often lacking. Epitaxial aluminium thin films were deposited on (0001) sapphire substrate by electron beam evaporation technique with different deposition parameters to establish a template based methodology for obtaining specific tilt GB types. EBSD measurements were employed to characterize the global GB structure, type and fractions present in the films. Cross-sectional view TEM samples from different films were prepared using plasma (Xe) focused ion beam (FIB) to systematically study the growth of aluminium on sapphire. Also, plan-view samples having Σ13b, Σ19b, and Σ7 GBs were extracted. First results of the local atomic structure of these GBs using advanced transmission electron microscopy techniques will be reported and discussed.

MM 30.4 Tue 18:15 P4

Fractal abnormal grain growth in nanocrystalline Pd(Au): correlation between Au concentration, hardness and microstructure — •Markus Fischer[1], Raphael Zeller[1], Christian Braun[2], Jonas Endres[1], Rainer Birringer[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

With an average grain size below 100 nm, nanocrystalline materials often manifest enhanced mechanical properties, like higher strength or hardness, but the fine microstructure tends to go hand in hand with poor stability against grain growth. The latter generally starts at much lower temperatures than in coarser-grained specimens of the same material, and the coarsening process itself can proceed in an abnormal manner. In nanocrystalline $\mathrm{Pd_{90}Au_{10}}$ alloys prepared by inert gas condensation (IGC), such abnormal growth leads to an impinged state of grains exhibiting highly irregular shapes, the perimeters of which are characterized by a box-counting fractal dimension of ~ 1.2; this value is significantly greater than the dimension of unity for grain perimeters of conventional samples [1]. However, when Au-free nanocrystalline Pd is prepared by IGC, grain growth leads to smaller grains at impingement and smoother boundaries. To shed light on the role played by Au atoms during the coarsening of nanocrystalline Pd(Au), we have searched for correlations between grain morphology, local hardness (as revealed by nanoindentation) and the Au concentration.
[1] C. Braun *et al., Scientific Reports* **8** (2018) 1592

MM 30.5 Tue 18:15 P4

Fractal abnormal grain growth in nanocrystalline Pd(Au): a result of abnormal growth triggered by pinning centers? — •Raphael Zeller[1], Tobias Okker[1], Karina De La Torre[1], Christian Braun[2], Mingyan Wang[1], Rainer Birringer[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

Although physical models have succeeded in explaining the migration of grain boundaries in polycrystals having micrometer-sized grains, our understanding of grain growth in nanocrystalline materials is still rudimentary. For example, in nanocrystalline Pd–10 at% Au produced by inert gas condensation, microstructural coarsening is found to be doubly abnormal, with a subpopulation of rapidly growing grains sending forth “tentacles” into the surrounding matrix, encircling nearby grains and then consuming them; moreover, the perimeters of the resulting grains resemble those of fractal objects. Computer simulations have ruled out two possible mechanisms for this fractal abnormal grain growth (AGG): coalescence via grain rotation and boundary migration according to highly anisotropic (reduced) mobilities. In Monte Carlo simulations reported by Holm *et al.,* pinning particles were observed to trigger explosive AGG. Since our nanocrystalline Pd–10 at% Au samples contain a small volume fraction of pores that could act as pinning centers, we performed phase field simulations to determine the pinning force per pore and to search for a connection between boundary fractality and the size and spatial distribution of pinning centers.

MM 30.6 Tue 18:15 P4

Structural relaxation in nanocrystalline Pd90Au10 — •Christian Braun, Michael J. Deckarm, Nils Boussard, and Rainer Birringer — Experimental Physics, Saarland University, Germany

The synthesis of nanocrystalline (nc) materials – either by the top-down or bottom-up approach – results in non-equilibrated material states that strongly depend on the specific sample synthesis and preparation history. Energy in excess to the crystalline ground state is stored in the disordered core regions of the interfaces as well as strain energy associated with crystal lattice distortions and the presence of lattice defects. Hence, annealing of these materials at temperatures below grain growth induces structural relaxation/aging and as a consequence the core structure of interfaces and the material properties change with time. In nc materials, structural relaxation has to be considered as a heterogeneous process due to the complex structure of the grain boundary (GB) network which can be imagined as an assemblage of structural units characterized by a site-specific deviation from local equilibrium. To adapt these heterogeneous nature of the GBs, we employed a distributed reactivity model to analyze volume relaxation of nc Pd90Au10. This approach partitions the overall relaxation process into a set of independent and parallel reactions and was applied to a set of dilatometer data captured under different time-temperature protocols to probe the spectrum of potential barriers the material has to overcome on its way to equilibrium. Furthermore, we analyzed the corresponding change in mechanical properties and microstructure.

MM 30.7 Tue 18:15 P4

Correlative study of grain boundary segregation in nanocrystalline copper–nickel alloys — •Felix Fischer, Rüya Duran, Guido Schmitz, and Sebastian Eich — Institute for Materials Science, University of Stuttgart, Germany

Nanocrystalline material properties are dominated by grain boundaries (GB). In nanocrystalline copper–nickel alloys, which have high corrosion resistance, thermal conductivity, and fabricability, segregation of copper to GBs is energetically preferred and was previously quantified in simulations by Molecular Dynamics using a new embedded-atom alloy potential. In these simulations, the values for the solute excess depend highly on the GB structure. Comparison to experimental data is required, thus correlative transmission electron backscattering diffraction (t-EBSD) and atom probe tomography (APT) measurements are carried out on prepared nanocrystalline tips.

t-EBSD allows an evaluation of the grain orientations and thus the GB types, while APT gives an atomically-resolved digital reconstruction of the measured tip. Combing these two methods, the segregation of copper to GBs can be correlated to the GB type, alloy concentration as well as the annealing temperature and furthermore compared to the simulated segregation.

Experimental as well as simulated segregation curves will finally be compared and described by a previously developed model for interface segregation. The change in interface formation energy based on the new model will be predicted.

MM 30.8 Tue 18:15 P4

Abnormal grain growth in Al(Cu) assisted by Zener pinning — •Maria Hohm, Raphael Zeller, Mingyan Wang, and Carl E. Krill III — Institute of Functional Nanosystems, Ulm University, Germany

Abnormal grain growth occurs during the heat treatment of polycrystals when a subpopulation of crystallites undergoes rapid growth at the expense of neighboring grains, leading to a bimodal grain size distribution. In some cases, abnormal grain growth appears to be triggered by grain boundaries interacting with second-phase particles, a process called Zener pinning. Although of considerable technological importance, there is still no consensus regarding the mechanism(s) underlying abnormal grain growth assisted by Zener pinning; indeed, most experimental studies of the phenomenon have been carried out on sample sections or thin films, for which the free surface is a complicating factor. The latter limitation can be circumvented by 3D characterization techniques like diffraction-based x-ray microscopy, which are able to assess the size and morphology of grains, the lattice misorientation at grain boundaries and the distribution of pinning particles throughout a bulk specimen. From such data, we aim to identify how pinning particles initiate and govern abnormal grain growth in Al(Cu) alloys.

MM 30.9 Tue 18:15 P4

About the atomic structure of copper grain boundaries — •Lena Frommeyer, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The atomic structures of grain boundaries (GBs) as interfaces between two crystals are determining microscopic and macroscopic properties of a material. So far, GBs were mostly studied by atomistic simulations and only few experimental studies exist, investigating pure high angle GBs on an atomic level. Recent studies of pure Σ19b [111] tilt GBs in copper showed that a GB can undergo phase transformations and different atomic structures can coexist, both in symmetric and asymmetric GBs. Furthermore, two symmetric variants of the Σ19b GB were observed, having different structural units. They also show a different behavior in compensating for inclinational deviations.
In this work, the same system is used, but a different GB, the Σ37c [111] tilt GB, is analyzed. As for the Σ19b GB, two different symmetric variants are observed and their atomic structures are studied by aberration-corrected transmission electron microscopy. Furthermore, asymmetric variants are investigated to analyze their behavior in compensating for deviations from the symmetric GB plane inclination. By comparing the results to the Σ19b GB, primary conclusions can be drawn whether structural units of symmetric GBs and their asymmetric variants are unique features of specific GBs or if the relation follows a generic concept.

MM 30.10 Tue 18:15 P4

Effect of residual stresses on dislocation nucleation and motion in lamellar TiAl alloys — •Ashish Chauniyal and Rebecca Janisch — ICAMS, Ruhr Universität Bochum

Residual stresses are present within many microstructures due to lattice mismatch, curvature effects and/or processing history. These residual stresses are a known cause for microyielding and localized plasticity. In this work we study the effect of residual stresses on dislocation nucleation and motion using a two phase TiAl lamellar system. The lattice mismatch between hexagonal $\alpha_2(Ti_3Al)$,face centered tetragonal $\gamma(TiAl)$ phases creates coherency stresses in individual phases. These residual stresses are a known cause for microplasticity in lamellar TiAl. In this work we carry atomistic simulations of α_2/γ bilayers with a dislocation nucleator in γ phase which emits dislocation loops during deformation. Using this framework, we study the mechanism of emission, propagation and interface interactions of dislocations in a α_2/γ bicrystal, in correlation with coherency stresses present within the lamellae.

MM 30.11 Tue 18:15 P4

Mechanical testing of SAC soldered micro- and nanowire joints — •Samuel Griffiths and Guido Schmitz — Chair of Materials Physics, Institute for Material Science University of Stuttgart, Germany

Joining is a ubiquitous component of many modern macro- and microscopic technologies, and as such joints continue to be miniaturized, it becomes increasingly necessary to evaluate the effects of miniaturization on the mechanical properties of the structural materials. Wires are fundamental building blocks which have been extensively examined for their promising electrical/surface properties - considered for use in different micro and nano devices. Quantifications of their mechanical properties although remains limited.

Most fundamental to understanding the mechanical strengths and limitations of nanowires, is determining their dependency on diameter. Here, we present our creative methodology for mechanically testing Cu micro-/nanowires soldered to substrates with SAC to initially determine the weakest link. Additionally, our preliminary tensile results are presented in dependence of diameter. Experiments were conducted in an environmental SEM including both in-situ soldering and mechanical testing under constant temperature conditions. The phenomenological reasoning for the size dependency is also alluded to.

MM 30.12 Tue 18:15 P4

Microstructural and mechanical investigation of magnetic impulse welds of Aluminium and Copper — •David Stein[1], Maximilian Gnedel[1], Sven Winter[2], and Ferdinand Haider[1] — [1]Chair of Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg (Germany) — [2]Fraunhofer-Institut für Werkzeugmaschinen und Umformtechnik, IWU, Reichenhainer Straße 88, 09126 Chemnitz, Germany

Magnetic impulse welding (MPV) is one of the few methods that allows joining different kinds of metals with significantly differing melting temperatures. It is conducted by colliding two metal sheets at high velicities. A sound joint without embrittlement effects or the formation of critical amounts of intermetallic phases can be produced. The Al-Cu system is relevant for a variety of reasons. With the rise of electromobility, the need for cheap and light conductors like aluminum to be connected to copper is high. Furthermore, the results of the investigation of the joining mechanism between Al and Cu are relevant for systems like Al-Ti and Al-Fe, etc., whose welds are required for lightweight construction. The joining mechanisms of Al-Cu welds were mainly analyzed using scanning electron microscopy. The relevance of the occurring small amounts of intermetallic phases is determined by growing them via a heat treatment and comparing tensile testing results of heat treated and untreated welds. If a thin surface layer melts and resolidifies during the process, can be investigated with EBSD. With a variation of the process parameters the influence on the resulting microstructures and interfacial morphology has been studied.

MM 30.13 Tue 18:15 P4

Fracture Matching of Metals in Forensic Science — •Jens Balzer, Bert Weimar, Horst Katterwe, and Werner Deinet — Kriminaltechnisches Institut, Bundeskriminalamt, 65173 Wiesbaden

The comparison of marks caused by firearms and tools as well as of marks on fracture surfaces is of great importance in forensic sciences. Very often a forensic laboratory is asked to prove whether two or more pieces of a broken metal originally were part of one and the same object. Examiners magnify the marks using comparison light microscopes or comparison scanning electron microscopes. In a pattern fit analysis the matching is based on characteristic features of the fracture surface. Sometimes the question arises whether the degree of similarity is sufficient to make the statement that the two broken pieces were originally one.This corresponds in the toolmark case to the question, if two marks were produced by the same tool. For these, efforts have been made to obtain objective criteria for an identification using probability theory models. References: 1) Voss-de Haan, Katterwe, Simross *Physik in der Kriminaltechnik*, Physik Journal 2, 35, 2003; 2) Katterwe, Körschgen, Ahlhorn *Proceedings Marks*, ISBN 3-00-009338-9, Berlin 2001; 3) Katterwe *Fracture Matching*, AFTE Journal 37, 229, 2005; 4) Weimar, Katterwe, Braune *Formspuren* in Widmaier *Strafverteidigung*, Beck 2014; 5) Katterwe, Braune, Körschgen, Radke, Weimar *Comparison SEM in Forensic Science*, AFTE Journal 41, 283, 2009; 6) Stone *Probabilistic Model of Fractures in Brittle Metals*, AFTE Journal 36, 297, 2004; 7) Deinet, Katterwe *Probability Models*, AFTE Journal 39, 4, 2007.

MM 30.14 Tue 18:15 P4

Plane wave scattering on Janus spheres — •Jochen Wauer[1] and Tom Rother[2] — [1]Hochschule Neubrandenburg, University of Applied Sciences — [2]German Aerospace Center(DLR), Remote Sensing Technology Inst., Neustrelitz

Janus spheres are objects of growing interest in different fields of technology. They can be used in medicine for a precise drug positioning, and they hold an enormous potential for the development of new and active materials, just to mention only two applications of recent interest in nanotechnologies. Some of those Janus spheres are still industrially manufactured. It must be noted, however, that there exists a certain lack of knowledge about the scattering behavior of such objects although it might be of some interest not only for diagnostic purposes but also for discovering new applications. We present the application of the T-matrix method to solve the scattering problem of a plane electromagnetic wave on a dielectric sphere the surface of which is partially covered with a perfect metal. Additionally, the scalar scattering problem, i. e. the scattering of acoustic waves on different types of Janus spheres will be discussed. First results are presented, and an interesting effect for specially oriented Janus spheres at lower size parameters is discussed.

MM 30.15 Tue 18:15 P4

A school badge based on scalable structural color — •Shiyao Jia, Yudie Huang, Yi Wang, Wenxin Wang, Zhihang Wang, Jiaxu Chen, and Fanzhou Lv — Harbin Engineering Unversity,Harbin,China

The researches on alumina membrane already has hundreds of years, and owing to its highly ordered honeycomb structure, anti-corrosion, transparencyand mechanical properties, the alumina membrane has become a hot spot in nanotechnology in these years. Here, the optical interference at the interfaces of alumina membrane is used to selectively reflect the light and present the structural color, based on this theory, we made a vivid and colorful school badge. The thickness of alumina membranes are regulated by controlling the anodizing conditions precisely. Different light with specific frequency can be reflected by changing the thickness of alumina membranes, thus demonstrating the relevant structural color on corresponding areas and presenting the picture of school badge, which can be further developed as a nanophotonic device for sensing.

MM 30.16 Tue 18:15 P4

Oriented and isotropic electrospun magnetic nanofibers - experiment and simulation — •Timo Grothe[1], Jan Lukas Storck[1], Al Mamun[1], Marah Trabelsi[1,2], Michaela Klöcker[1], Christoph Döpke[1], Lilia Sabantina[1], Tomasz Blachowicz[3], and Andrea Ehrmann[1] — [1]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany — [2]Ecole Nationale d'Ingénieurs de Sfax, Sfax 3038, Tunisia — [3]Silesian University of Technology, Institute of Physics - Center for Science and Education, 44-100 Gliwice, Poland

Due to their strong shape anisotropy, magnetic nanofibers are of high interest in basic research as well as in spintronics, neuromorphic computing, for data storage, etc. Besides typical methods to prepare magnetic nanofibers, such as vapor growth, focused-ion-beam milling, or template-based methods, electrospinning allows for creating magnetic nanofiber mats [1].

Electrospun magnetic nanofibers, however, impose new challenges on micromagnetic simulations due to their varying diameters and bending radii. On the other hand, to allow for comparing simulated magnetization reversal processes with experimental findings, it is necessary to optimize the distribution of magnetic particles in the nanofibers.

Here we discuss different possibilities to tailor nanofiber diameters and shapes, influence the distribution of magnetic nanoparticles in the fibers as well as the nanofiber orientation inside the mat, and model static and dynamic properties of idealized and real nanofiber networks.

[1] C. Döpke et al., Nanomaterials 9, 92 (2019)

MM 30.17 Tue 18:15 P4

Comparison and analysis of ultra-narrow gaps fabricated by electron and helium ion beam lithography — Hao HU[1,2], Monika Fleischer[2], and •Pierre-Michel Adam[1] — [1]Universite de Technologie de Troyes, 12 Rue Marie Curie, CS42060, 10004 Troyes Cedex, France — [2]Institute for Applied Physics and Center LISA+, Eberhard Karls University Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Metal nanostructures with ultra-narrow gaps, which enable strong field enhancements in plasmonic structures, have attracted widespread attention in physics, chemistry, and biology. However, fabricating ultranarrow nanogaps is still challenging at present, and controllable gap size, accurate dimensions, and scalable fabrication are desired for further applications. The most common methods for fabricating nanogaps arrays are electron beam lithography (EBL) and focused ion beam (FIB) milling. Depending on the difference of cross-linking reaction and degradation reaction occurring under the electron beam, the photoresist can be classified into two types: positive tone and negative tone. FIB can be divided into He-ion and Ga-ion beam depending on the ion source used. In this study, we provide a comparison of nanostructures fabricated with different methods including different types of EBL and FIB. By varying the fabrication methods of the nanostructures, we aim to find optimized approaches for fabricating ultra-narrow nanogaps.

MM 30.18 Tue 18:15 P4

Magnetoresistance of ruthenium nanogranular wires — •Nikolai Mai[1], Thomas Heinzel[1], Mihai Cerchez[1], Shibesh Dutta[2], Anshul Gupta[2], Shreya Kundu[2], Giacomo Talmelli[2], Florin Ciubotaru[2], Zsolt Tokei[2], and Christoph Adelmann[2] — [1]Heinrich Heine University Düsseldorf, Universitätsstr. 1, 40225, Düsseldorf — [2]Imec, 3001 Leuven, Belgium

Ruthenium is a promising candidate to replace Cu for metallic interconnects as electronics continues to scale down. Although the resistivity of Ru is less dependent on the thickness of the interconnect than that of Cu, the scaling problem in this case manifests with increased resistivity as the size of the interconnect becomes comparable to the size of the grain and to the mean free path. Here we present longitudinal and transversal magnetoresistance measurements and IV characteristics of Ruthenium nanogranular wires discussing the role of the grain-interface in the Ru-resistivity.

The wires with a cross section less than $150\,\mathrm{nm}^2$ were obtained by a conformal atomic layer deposition of a 10 nm thick Ru film on SiO_2 cores (height 25 nm and width 300 nm) patterned on 300 mm Si (100) wafers, followed by an anisotropic reactive ion etch. The wires were protected by $SiN_x/SiO_2/SiN_x$ passivation layer, whereas the Al contacts were formed after passivation opening at the ends of the wires. The samples were at 420°C for 20 mins in forming gas.

MM 30.19 Tue 18:15 P4

Effect of Interfaces in the Oxide Transport Process in Platinum Coated Porous Frameworks of Yttria-Stabilized Zirconia (YSZ) — •Michele Bastianello[1], Jan-Ove Söngen[1], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Institute of Experimental Physics I, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Institute of Physical Chemistry, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 17

Oxygen permeation membranes are of high interest for the production of pure oxygen. Such membranes need to transport not only oxygen ions but also the electronic charge carriers making mixed conducting oxide ceramics necessary. Research focusses mostly on multi-phase oxidic mixture or on high amounts of noble metals in oxide ceramics to achieve high mixed ionic and electronic conductivity. As an alternative approach, we hereby present the preparation of nano-structured composite materials using pulsed laser deposition (PLD) combined with atomic layer deposition (ALD). In particular, using PLD porous YSZ thin films were prepared and their surface was coated homogeneously with about 36 nm of Platinum using ALD. The transport properties of the composites were investigated using electrochemical impedance spectroscopy. To elucidate the influence of the interfaces, a series of multilayered YSZ-Pt-YSZ samples were prepared using PLD in order to obtain a fully controlled model system for comparison.

MM 30.20 Tue 18:15 P4

Optimization of structural and electrochemical properties of $LiNiO_2$ thin film cathodes — •Juri J.E. Becker, Fabian Michel, Hendrik Hemmelmann, Angelika Polity, and Matthias T. Elm — Center for Materials Research, Gießen, Germany

Due to its higher energy density layered lithium-nickel(III)-oxide (LNO) is a possible alternative to lithium cobalt oxide, which is used as cathode material in lithium-ion batteries (LIBs). However, LNO suffers from thermal instability as well as the fact that Ni^{2+}-ions have the tendency to substitute Li^{+}-ions during delithiation. To investigate the structural and electrochemical properties of LNO in more detail, thin films were prepared as model electrodes using radio frequency magnetron sputtering. For this purpose, a LNO target was pressed and thin films were deposited on a c-sapphire|platinum substrate. The influence of the growth temperature on the structural properties during the sputtering process was examined. At higher temperatures the crystallinity of LNO is increased which allows a better lithium-ion diffusion during the intercalation process. Pouch-cells were built using the deposited cathodes. Electrochemical measurements with a potentiostat reveal phase transitions occuring during the cycling process.

MM 30.21 Tue 18:15 P4

Ti3C2/MoS2 composite as anode material for lithium-ion batteries — •Peng Guo[1,2], Yuquan Wu[1], Lennart Singer[1], Peter Comba[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]Inorganisch-Chemisches Institut, Universität Heidelberg, Germany

MXene, represented by Ti3C2, has received increasing attention when applied as anode material for lithium-ion battery due to its superior conductivity and hydrophilicity. Since the application of MXene is limited by its low capacity, in this work, a PDDA-assisted electrostatic attraction method was used to assemble a Ti3C2/MoS2 composite. The microscopic morphology, crystalline features and microstructure of the Ti3C2/MoS2 composite materials studied by X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM) are reported. Electrochemical studies reveal a specific capacity of 747 mAhg-1, at 400 mAg-1, of the Ti3C2/MoS2 composite electrode which notably increases to 776 mAhg-1 after 30 cycles.

MM 30.22 Tue 18:15 P4

Polypyrene tetraone (PPTO) as cathode material for lithium-ion batteries — •Jonas Spychala[1], Yuquan Wu[1], Lucas Ueberricke[3], Michael Mastalerz[3], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Centre for Advanced Materials, Heidelberg University, Germany — [3]Organisch-Chemisches Institut, Heidelberg University, Germany

Covalent organic frameworks (COFs) have emerged as promising candidates for cathode materials in lithium-ion batteries, due to their superior conductivity, electrochemical stability and structural richness. In order to assess the feasibility of Polypyrene tetraone (PPTO) for electrochemical energy storage, we have investigated its electrochemical properties by means of cyclic voltammetry (CV), galvanostatic cycling (GCPL), and electrochemical impedance spectroscopy (EIS). Cyclic voltammetograms show two characteristic redox pairs, at 2.4 V and 2.8 V, respectively, with small overpotentials. In comparison to the monomers which capacity amounts to 70 mAhg^{-1} in the initial cycles, PPTO delivers significantly increased capacities of 140 mAhg^{-1}. This indicates that higher carbonyl utilization is achieved by polymerization. The capacity retention in PPTO by cycle 10 is 96% and 70% by cycle 50. The effects of different porosities and electrode fabrication procedures are discussed.

MM 30.23 Tue 18:15 P4

Phase transformation in Li4+xTi5O12 probed optically — •Yug Joshi, Robert Lawitzki, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Stuttgart, Germany

The mechanism and the kinetics of the phase transformation from spinel structured Li4Ti5O12 to rock-salt type Li7Ti5O12 is studied by utilizing the electrochromic properties of the material. Thin films of Li4Ti5O12 are deposited on platinum-coated substrates using rf-ion beam sputtering. In-situ and ex-situ optical spectroscopy (in reflectance geometry) is performed along with electrochemical characterization. In-situ measurements demonstrate the reversible electrochromic behavior of the deposited thin films and the effect of the change of lithium content on the reflectance spectrum. The kinetics of the phase transformation is examined by probing the lateral diffusion lengths of lithium, optically revealed by the drastic blue color of the lithium-rich rock salt phase. Ex-situ measurements quantify the optical constants of the thin films for different charge states, by modeling the reflectance spectrum with a Clausius-Mossotti relation. The concentration dependence of the derived dielectric constants points out a fast lithium ion transport through the grain boundaries, thereby segregating a conductive lithium-rich phase at the grain boundaries. This is further confirmed by the change in the lateral diffusion lengths (reveled optically) with the varying grain sizes.

MM 30.24 Tue 18:15 P4

Template-Assisted Fabrication of Spectrum-Programmable Superlattice Photonic Crystals for Efficient Solar Energy Harvesting — •Zhiqiang Zeng, Rui Xu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98693, Ilmenau, Germany.

Superlattice photonic crystals (SPhCs) possess tremendous potentials as building blocks for high-performance solar thermal conversion systems because of their great flexibility in optical manipulation. For practical utilization of SPhCs as solar absorbers, the key points are to fabricate large-scale highly-ordered SPhCs and to realize spectrally-programmable selective light absorption spectra. In this work, wafer-scale nickel (Ni) SPhCs are fabricated by structurally replicating alumina templates comprising two sets of nanopores (NPs) and nanoconcaves (NCs). Both self-aligned sets of NPs and NCs are simultaneously formed during the anodization of surface-patterned aluminum foils, consequently avoiding otherwise multi-step lithography and resulting in large-scale uniformity. The as-replicated Ni SPhCs demonstrate omnidirectional polarization-independent selective light absorption spectra whose cutoff wavelength can be precisely programmed in the spectral range of ~600 to ~1500 nm. Below the cutoff wavelength all absorption efficiencies are enhanced to over 90% due to surface plasmon resonance and cavity resonance stemming from both NCs and NPs. All these advantages in optics and fabrication qualify Ni SPhCs as excellent candidates of solar absorbers for practical utilization.

MM 30.25 Tue 18:15 P4

Non-adiabatic time-optimal edge mode transfer on mechanical topological chain — •Ioannis Brouzos[1], Georgios Theocharis[1], Ioannis Kiorpelidis[1], and Fotios Diakonos[2] — [1]Laboratoire Acoustique Universite Mans — [2]University of Athens

We show that it is possible to successfully transfer topologically protected edge modes across a mechanical chain, with non-adiabatic optimal control schemes, in a time even shorter than their own period. The proposed protocols vastly outperform the adiabatic ones, both in time-scales and in robustness against disorder. Our control schemes possess non-adiabatic time intervals during which driving frequencies exceed characteristic frequencies of the system, shift the value of adiabatic invariant, and exchange a great amount of energy. As a bonus feature and in contrast with quantum chains, ultrafast pumping in classical chains is accompanied with amplification of the edge mode. Introducing non-adiabatic pumping of topologically protected states aims to challenge common approaches in this emerging field.

MM 30.26 Tue 18:15 P4

Atomistic investigation of the LLZO / Li metal interface for all-solid state batteries — •Lisette Haarmann and Karsten Albe — Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt

In order to achieve maximal energy densities in all solid state Li ion batteries (ASSB), the introduction of a metallic Li anode is crucial. However, the interface kinetics between Li metal and the solid electrolyte is mostly unexplored and an atomistic picture is still missing. Therefore ab-initio calculations based on density functional theory (DFT) are carried out in order to investigate the lithium transfer over this interface.

Aluminium doped $Li_7La_3Zr_2O_{12}$ (LLZO) is considered as a model system due to its stability against lithium metal and its minimal intrinsic interface resistance. Jump processes of lithium between the metal (atomic state) and the electrolyte (ionic state) and the accompanying charge transfers are investigated both with Nudged Elastic Band (NEB) calculations and ab-initio Molecular Dynamic (AIMD) simulations.

While the former provides activation energies for the jump processes, the latter allows the investigation of structural rearrangements at the interface above 0 K, as well as the calculation of lithium diffusion coefficients and preferred transport directions.

Combining the information of both approaches, the energy landscape of the LLZO / Li metal interface is constructed providing information on the lithium transport in an ASSB.

MM 30.27 Tue 18:15 P4

Hybrid Functionals in an all-electron FLAPW basis: challenges imposed by exa-scale supercomputers — •Matthias Redies[1,2], Gregor Michalicek[1], Christian Terboven[3], Daniel Wortmann[1], Matthias Müller[3], and Stefan Blügel[1] — [1]Forschungszentrum Jülich and JARA — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]IT Center, RWTH Aachen University, 52074 Aachen, Germany

Hybrid exchange-correlation functionals facilitate some of the most accurate DFT calculations and are especially important in systems, where traditional exchange-correlations functionals fail, such as oxides. However, this accuracy comes at a large computational cost. Until recently these calculations have been restrained to small system, due to the excessive demand for computing resources. This large computational demand makes hybrid functionals a suitable problem for the next generation of supercomputers.

On this poster we are going to present how we parallelize and adapt the FLEUR [1,2] code, an all-electron FLAPW implementation developed in Forschungszentrum Jülich, to perform hybrid functional calculations efficiently on next generation supercomputers and present a path towards utilizing heterogenous computing architectures.

This work was supported by the EU-CoE MaX [3], JARA-HPC and the JARA-CSD School for Simulation and Data Science (SSD).

[1] www.flapw.de [2] Friedrich *et al.*, J Phys: Condens Matter. **24(29)**:293201. [3] www.max-centre.eu

MM 30.28 Tue 18:15 P4

Nonequilibrium dynamics of laser excited SiC: Description of Laser excited SiC with the help of an electronic temperature dependent interatomic potential — •Malwin Xibraku, Bernd Bauerhenne, and Martin Garcia — Heinrich-Plett-Straße 40, 34132 Kassel

Silicon carbide (SiC) nanocrystals are of great interest in medicine, because of their pleasant properties, such as biocompability, high chemical and thermal stability. These nanocrystals can be very well generated using ultrashort laser pulses. Density Functional theory (DFT) has proven to be a appropriate tool to describe the influence of ultrashort laser pulses on solids due to the accurate quantum mechanical treatment of electrons. Due to the fact that 48 million particles are already contained in a cube SiC of side length 100 nm, such a system cannot be computed with DFT. Therefore, the aim of this work is to describe the forces between the atoms in the SiC cube by an effective electronic temperature (Te) dependent interatomic potential. Te is taken into account for including the effect of the laser-excited electrons. Recently, we found such a potential for silicon (Si) and carbon (C). In this work, a potential for siliconcarbite (SiC) was constructed. This potential reduces to the existing potentials for silicon (Si) or carbon (C), if only silicon (Si) or carbon (C) particles are present, respectively.

MM 30.29 Tue 18:15 P4

Molecular dynamics study of impact welding processes — •Benedikt Philipp Eggle-Sievers, Tobias Stegmüller und Ferdinand Haider — Universität Augsburg, Institut für Physik, Universitätsstraße 1 86159 Augsburg

Impact welding processes like explosive welding or magnetic pulse welding allow for the joining of different materials in a fast and reliable fashion. In the presented work, such joints between Al and Cu are investigated by the means of molecular dynamics simulations. The process of impact welding is divided into two stages, the loading and the unloading stage. The MD model consists of two plates forming a typical impact angle between 5° and 30°. Besides the impact velocity, typically being several hundreds of meters per second, the angle is the parameter to vary. Another investigated phenomenon is the formation of a jet between both plates. It is an open question of ongoing research, whether the jetting can be traced back to the surrounding atmosphere, or to flaking and local melting of the material whilst the collision. In the presented work, the influence of the brittle oxide layer on the Al-surface is considered, requiring advanced potentials with the capability to capture the properties of metallic as well as of covalent–ionic bonds.

MM 30.30 Tue 18:15 P4

Ab Initio **Molecular Dynamics Simulations of Chemical Processes at the Crack Tip** — •Tobias Müller and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Fracture of materials takes place in an environment, usually air or liquid water. When a crack propagates, the newly created surfaces become exposed to the molecules of the surrounding gas phase or liquid, e.g. oxygen and water, which leads to a series of chemical processes. For example, the molecules can attack a stretched bond at the crack tip, giving rise to chemically activated bond breaking and resulting in subcritical crack growth and stress corrosion cracking. In order to encompass the complex chemical interplay between bond breaking at the crack tip and the adsorption/bond saturation with molecules from the environment, unbiased and accurate quantum-chemical methods are needed. Here we show first *ab initio* molecular dynamics simulations for silicon to study stress corrosion cracking by subcritical loads. A series of Car-Parrinello molecular dynamics (CPMD) simulations were performed with different loads and for crack tips exposed to hydrogen, oxygen or water.

MM 30.31 Tue 18:15 P4

Development of an analytic bond-order potential for Fe-Co — •Aleksei Egorov, Aparna Subramanyam, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The growing demand for soft magnets and the potential for magnetic topological structures continue to draw attention to Iron-Cobalt (Fe-Co) alloys. The description of the magnetic degrees of freedom for the calculation of the phase diagram and microstructural properties are still a challenge for atomistic simulations. Quantum-mechanical approaches capture the details of the magnetic interactions, but are typically too computationally expensive for large scale simulations or extensive sampling of spin space at finite temperature. The computationally less demanding classical approaches usually cannot provide a reliable description of the influence of magnetism. Here we report the development of an analytic bond-order potential (BOP) for Fe-Co that provides a robust description of magnetism in large-scale simulations.We parameterize the analytic BOP with reference data obtained by density functional theory (DFT) calculations using two parameterization strategies: i) chemical morphing of an existing BOP for Co towards Fe by varying the band filling and ii) successive parameterization of the BOP parameters starting from DFT-based Hamitlonian matrix elements. We use the obtained BOP models to study the band filling trends of structural stability and the volume dependence of the magnetic moment. The results are compared to the available experimental and DFT data and analyzed with canonical band theory.

MM 30.32 Tue 18:15 P4

The Process for Creating A General-Purpose Machine Learned Potential for Silicon Carbide — •Harry Tunstall, James Kermode, and Gabrele Sosso — The University of Warwick, Coventry CV4 7AL, United Kingdom

SiC is a prototypical material for high temperature applications (e.g aerospace, automotive and thermoelectric) involving complex microscopic processes typically inaccessible to experiments. To gain insight into the functional properties of e.g. SiC nanostructures, computationally expensive quantum mechanical methods such as density functional theory (DFT) must be employed. This is because less computationally demanding methods are almost always not accurate enough. In fact, similar to Si and C alone, various empirical interatomic potentials have been developed for SiC, such as Tersoff or Stillinger-Weber. These potentials are designed to reproduce specific features of the material, at the expense of transferability to a wider range of functional properties.

The aim of this project is to build a general purpose interatomic potential for SiC (e.g using machine-learning regression, in the form of Gaussian approximation potentials (GAPs) and neural networks (NNs), starting from a DFT dataset of representative configurations), enabling accurate large scale simulations into defects and grain boundaries. The methodology for creating and maintaining a machine learning database for atomic systems from the ground up will be discussed, from the perspective of this ongoing project.

MM 30.33 Tue 18:15 P4

Density functional study of metal and metal-oxide (Cu, Ni, Co, Fe, Mn) nucleation and growth on the anatase TiO_2(101) surface — •Leila Kalantari, Fabien Tran, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology,Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

Experimental studies have shown the possible production of hydrogen through photocatalytic water splitting using metal oxide (MO_x) nanoparticles attached on anatase TiO_2 surface. In this work, we performed density functional theory calculations to provide a detailed description of geometry, electronic properties and catalytic sites. The adsorption of M_xO_y(M=Cu, Ni, Co, Fe and Mn) and (x = 5, y = 0-5) clusters on the TiO_2(101) surface has been studied using the PBEsol exchange correlation functional with a Hubbard correction (U). Various geometries of metals and metal-oxide have been investigated. It is found that, unsaturated 2-fold-coordinated oxygen sites may serve as nucleation centers for the growth of metal cluster and the adsorption of Ni atoms on the anatase surface is stronger than of other atoms. Energetically, the NiO cluster prefers the bridge site formed by 2-fold-coordinated oxygen atoms with an adsorption energy of 3.55 eV. We found that the Ni_nO_n adsorption energy remains about constant with cluster size n which makes the formation of bigger clusters plausible as confirmed by TEM images. Ni has a more stable configuration with less oxygen, while for other metals the adsorption energy remains almost constant or is reduced with less oxygen specially in Mn, which is in agreement with the experimental results.

MM 30.34 Tue 18:15 P4

Neural network for learning and predicting tight-binding parameters — •Till Hanke, Jürgen Henk, and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg

Tight-binding approaches have two major advantages: they allow for an intuitive interpretation of electronic structures and to perform large-scale electronic-structure calculations. However, parameter sets, either DFT-based or empirical, are often available only for simple bulk systems.

We report on artificial neural networks which can predict Slater-Koster tight-binding parameters for heterogeneous systems. The networks are trained using parameter sets for elemental materials. These sets will be used for electronic-structure and transport calculations (on the femtosecond timescale) for which accurate descriptions of complex interfaces are essential.

MM 30.35 Tue 18:15 P4

High-dimensional neural network potential for laser-excited materials — •Pascal Plettenberg, Bernd Bauerhenne, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

In recent years, machine learning techniques have been increasingly used to develop highly accurate representations of ground state or single excited state potential energy surfaces (PES) for large systems. Here, we want to develop such a machine learning potential to electronic temperature (T_e) dependent PES of solids excited by intense femtosecond laser pulses. Studying the effects of ultrashort excitation on the long-term (nanoseconds) and large-scale (hundreds of nanometers) dynamics of a material has not been possible so far, because ab-initio simulations are limited to a small number of atoms and short time scales. On the other side, T_e-dependent interatomic potentials, which can be efficiently used in large-scale simulations, are difficult to derive and often do not reach the required accuracy. In this work we investigate the possibility to fill this gap of simultaneous efficiency and ab-initio accuracy with a high-dimensional neural network potential including an electronic temperature dependency, which is implemented as an additional input node. We train the network to reference Density-Functional-Theory data of thin-film silicon and demonstrate its performance in molecular dynamics simulations.

MM 30.36 Tue 18:15 P4

Application of Machine Learning Interatomic Potentials to Carbon Nanostructures — •Tom Rothe[1], Erik Lorenz[1,2], Gustav Johansson[3], Fabian Teichert[1], Daniel Hedman[3], Andreas Larsson[3], and Jörg Schuster[1,2] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Luleå University of Technology, Luleå, Sweden

Machine Learning Interatomic Potentials (ML-IAPs) are a new class of non-empirical IAPs for atomistic simulations that are created using Machine Learning methods. Promising near quantum mechanical accuracy while being orders of magnitudes faster than first principle methods, they are the new "hot topic" in material simulation research.

This work investigates the state of the research in the field of ML-IAPs for simulation of carbon nanostructures (CNS). Publicly available ML-IAPs are used for simulation of defect induced deformation of carbon nanotubes. Comparing the results with previously published density-functional tight-binding results and our own empirical IAP geometry optimizations show that ML-IAPs can already be used for simulations of CNS. They are indeed faster than and nearly as accurate as first-principle methods.

We also present results for a new Neural Network-based ML-IAP trained on graphene, haeckelite, carbon nanotube, and fullerene structures, with and without defects.

MM 30.37 Tue 18:15 P4

a Neural Network Potential with electrostatic interaction — •Tsz Wai Ko and Jörg Behler — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, German

High-dimensional neural network potentials (HDNNPs), which represent one of the most frequently used types of ML potentials, construct the short-range energy as a sum of environment-dependent atomic energy contributions. In addition, long-range electrostatic interactions can be included employing environment-dependent atomic charges. Both contributions are determined using atom-centered radial and angular symmetry functions as local structural descriptors.

Here we present benchmark calculations for several model systems such as water molecules and Zinc oxide clusters using Density Functional Theory reference calculation

MM 30.38 Tue 18:15 P4

Machine-learning Driven Global Optimization of Atomic Surface Structures — •Sami Kaappa and Karsten Wedel Jacobsen — CAMD, Department of Physics, Technical University of Denmark, 2800 Kongens Lyngby, Denmark

Efficient global optimization of atomic structures is a long-pursued objective in material sciences since the required number of *ab initio* calculations is usually computationally infeasible. In this work, a machine-learning guided approach is utilized to model the potential energy hypersurface (PES) as a function of atomic coordinates, and the surrogate model is used to intelligently sample the search space for the global minimum in order to reduce the number of expensive DFT calculations. In the method, the translational and rotational symmetries as well as symmetries with respect to interchanging positions of alike atoms are naturally inherited by a global fingerprint, and both energy and force information of DFT calculations are used in the Gaussian process machinery to model the PES. We will present both the performance of the method in comparison to previously reported, similar procedures, and predicted global minima for certain atomic structures where the optimal atomic configuration is not trivial. Although DFT calculations are carried out here, we note that higher-level theories can be used as well to probe energies and forces of single structures, to be offered as training data for the model.

MM 30.39 Tue 18:15 P4

Symmetry-adapted Hamiltonian representations for machine-learning-based tight-binding parametrization — •Michael Luya[1] and Reinhard Maurer[2] — [1]Department of Mathematics, University of Warwick, Coventry, UK — [2]Department of Chemistry, University of Warwick, Coventry, UK

To tackle modern materials challenges, high efficient and accurate electronic structure methods need to be available that reliably predict the atomic structure, electronic and spectroscopic properties of materials at ever larger scales. Machine-learning methods have recently revolutionised the construction of interatomic potentials in computational materials science and are increasingly considered for the efficient construction of effective electronic structure methods such as tight-binding. Here we explore two-centre, three-centre and crystal field parametrisations of Hamiltonians in local basis representations that conserve important symmetries including rotational equivariance properties and permutational invariance. We show that this representation can accurately map on-site and off-site Hamiltonian contributions extracted from Density Functional Theory. We also investigate the physical significance of these parameters and the prospect of integration into deep-learning based parametrisation schemes.

MM 30.40 Tue 18:15 P4

X-ray reflectivity of thin films evaluated by neural networks — Thorben Finke and •Uwe Klemradt — II. Physik. Inst., RWTH Aachen University, Germany

X-ray reflectivity (XRR) is a widespread method for the structural analysis of thin films on the nanometer scale. We studied the application of a neural network based on Tensorflow for the evaluation of reflectivity curves from metal films of several 10 nm thickness on Si substrates. The focus was on the automatic fitting of layer thickness and surface / internal interface roughness. The network was trained using 900k simulated XRR curves and provided highly accurate results in subsecond computation time, resulting in thickness and roughness errors below 0.1 nm in 95% of the cases when applied to data not known to the network. The results will be discussed in the context of automatic fitting with minimum user interference and high-throughput experiments.

MM 31: Invited talk Spearot

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

Invited Talk MM 31.1 Wed 9:30 BAR 205

Importance of Dislocation Character Angle and Local Stress State Dependent Mobility Laws on Discrete Dislocation Dynamics Modeling of Plasticity in Aluminum — •Douglas Spearot[1], Khanh Dang[2], Darshan Bamney[1], and Laurent Capolungo[2] — [1]University of Florida, Gainesville, FL, USA — [2]Los Alamos National Laboratory, Los Alamos, NM, USA

In discrete dislocation dynamics (DDD) modeling, the motion of dislocation segments is governed by mobility laws that relate segment glide velocity to the resolved shear stress in the Burgers vector direction acting on the segment. These relationships make assumptions about the role of dislocation character angle and do not consider influences of non-Schmid stresses. Thus, the objective of this work is to derive new mobility laws for dislocations in Al using molecular dynamics (MD) simulations, which are necessary to improve the representation of the physics of dislocation motion in DDD modeling. Specifically, mobility laws for screw, 30 degree, 60 degree and edge dislocations are atomistically derived for different combinations of Escaig stress and stress normal to the (111) slip plane. MD simulations show that both phonon drag and radiative damping regimes are influenced by the presence of non-Schmid stresses, mainly through changes to the dislocation core structure. Model forms characterizing the mobility laws are incorporated into a DDD modeling tool. DDD simulations of dislocation network evolution show that the use of stress state dependent dislocation mobility laws provides changes to the plastic deformation path, leading to different final dislocation microstructures.

MM 32: Topical Session: Data Driven Materials Science - Materials Data Management (joint session MM/CPP)

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

Topical Talk MM 32.1 Wed 10:15 BAR 205

Automated atomistic calculation of thermodynamic and thermophysical data — •Jan Janssen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

A major challenge in predicting the properties of materials at realistic conditions is the accurate inclusion of finite temperature effects. Doing this on an ab initio level often requires complex simulation protocols. These complex protocols, which often couple several specialized codes, make a quantitative description of error propagation and uncertainty quantification a critical issue.

To handle this high level of complexity we have developed an integrated development environment (IDE) called pyiron[1] - http://pyiron.org. pyiron has been specifically designed to scale simulation protocols from the interactive prototyping level up to the high throughput level, all within the same software framework.

We highlight two recent success stories towards automated calculation of phase diagrams: We first discuss with the automated convergence for all key parameters in DFT codes, followed by the calculation of melting points with a guaranteed precision of better than 1K. These fully automated high-precision tools allow us to study trends over the periodic table in an efficient and systematic way. Examples how such high-throughput screenings allow to develop new strategies in designing materials will be given.

[1]: J. Janssen, et al., Comp. Mat. Sci. 161 (2019)

MM 32.2 Wed 10:45 BAR 205

Big data in materials science: Status of and needs for metadata and ontologies — •Maja-Olivia Lenz, Luca M. Ghiringelli, Carsten Baldauf, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In recent years, the amount of data in materials science has increased exponentially. Consequently, new ways to store and annotate data are necessary to ensure findability, accessibility, interoperability and re-usability, i.e. to fulfil the FAIR principles [1], and to do efficient, good and new science. Data describing and characterizing other data are called metadata. Often, the materials science community has no clear distinction between data and their metadata as it depends on the intended use of the data. In this talk, we present the NOMAD MetaInfo [2], a general descriptive and structured metadata scheme for materials simulations. Ontologies represent the next step on the semantic ladder, as they enrich pure (meta)data structures by relations and thereby enable semantic and syntactic interoperability between different software agents, people, and organizations. In fact, the NOMAD MetaInfo includes a number of relations between concepts and therefore goes beyond the simple metadata picture. It can be interpreted as a light-weight ontology and thus can easily be connected to other ontologies like the European Materials and Modeling Ontology, EMMO. We give an introduction to ontologies, explain why they are useful, and outline their role and current status in materials science.

[1] M. Wilkinson, *et al.*, Sci Data 3, **160018** (2016).

[2] L. M. Ghiringhelli *et al.*, npj Comput. Mater. 3, **46** (2017).

MM 32.3 Wed 11:00 BAR 205

Benchmarking neural networks on sequence-determined polymer transport through lipid membranes — •Marco Werner[1], Yachong Guo[2], and Vladimir Baulin[3] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Germany — [2]National Laboratory of Solid State Microstructure, Department of Physics, Nanjing University, China — [3]Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, Spain

We consider the transport of amphiphilic polymers through lipid membranes by passive diffusion as a function of the sequence of hydrophilic and hydrophobic building blocks. Massively parallel Rosenbluth sampling of polymer conformations is performed to estimate polymer translocation times through a membrane for all 2^N sequences and chain lengths $N \leq 16$. Our results confirm that smallest translocation times are found for polymers with balanced fraction of hydrophilic and hydrophobic units, and containing short blocks. Sequence-complete databases deliver an important ground truth for benchmarking machine-learning models against training data restrictions and biases. We demonstrate that multi-layer artificial neural networks show remarkable generalization performance when restricting the training data to relatively narrow windows of translocation times. The results indicate that relevant sequence patterns and their physical effect are approximated based on the restricted training set, however, accuracy drops towards unexplored corners in sequence space.

MM 32.4 Wed 11:15 BAR 205

Analysis of Materials Structural Representations for Machine Learning Interatomic Potentials — •Berk Onat[1], Christoph Ortner[2], and James Kermode[1] — [1]School of Engineering, University of Warwick, Coventry, United Kingdom — [2]Mathematics Institute, University of Warwick, Coventry, United Kingdom

Representations of materials based on atomic structural environments have been used either in machine learning models to predict properties directly or as the core of machine learning interatomic potentials (MLIPs) to enable accurate simulations. Many MLIPs have been developed to translate atomic neighbourhood environments from atom positions to structural representations such as atom-centred symmetry functions, smooth overlap of atomic positions and atomic cluster expansion(ACE) with spherical harmonics. While use of these representations is becoming common practice for applications, the sensitivity of their structural mapping to the materials composition and whether their coverage of the hyper-dimensional space is over-determined or complete have not yet been fully analysed. In this presentation, we provide analysis of the invariance of the model transformation under translations and rotations as well as the sensitivity of descriptors to perturbations. A range of datasets extracted from the NOMAD Archive are used to assess the dimensionality of the representations. The outcomes of our analyses will be presented with discussions on the model sensitivities and their possible limitations. We further provide insights on our continuing affords to utilise structural representations in other models for data-driven materials modelling.

MM 33: Topical Session: Interface-dominated phenomena - Hydrogen at Interfaces

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

MM 33.1 Wed 10:15 IFW A

Effect of grain boundaries on self-diffusion and hydrogen diffusion in bcc iron — •Daria Smirnova, Sergei Starikov, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Bochum, Germany

Grain boundaries (GBs) are known to affect diffusion processes in most materials. In this work, we employed atomistic simulations to investigate how both self-diffusion and hydrogen diffusion processes are altered in the vicinity of various GBs in body-centered cubic (bcc) iron. The investigations were performed using accurate ab initio calculations based on density functional theory and large-scale molecular dynamics simulations with various interatomic potentials. We found that for symmetric tilt GBs the self-diffusion is mostly driven by interstitial atoms while in general GBs Fe atoms diffuse predominantly via an exchange mechanism that does not involve a particular defect and is similar to liquid diffusion. In most investigated cases, the self-diffusion along GBs is significantly enhanced compared to that in bulk. In contrast, the motion of H atoms along GBs is at ambient temperatures several orders of magnitude slower than the H bulk diffusion. This outcome is related to larger migration barriers in the distorted crystal structure of GBs, compared to a very low H migration barrier in bulk bcc Fe. We present temperature variations of diffusion coefficients for different GBs and compare the simulation predictions with available experimental data.

MM 33.2 Wed 10:30 IFW A

Ab initio analysis of hydrogen segregation and embrittlement at cleavage plains and at a grain boundary in bcc Fe — •Abril Azócar Guzmán, Jeongwook Jeon, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-Universität Bochum

Grain boundaries in ferritic microstructures play a dual role in the context of hydrogen embrittlement: on the one hand, they act as H traps and thus reduce the amount of mobile H in the system. On the other hand, exactly this trapping is expected to promote hydrogen enhanced decohesion at the grain boundaries. In order to influence the segregation process as well as the cohesive properties of interfaces in ferrite, one needs to understand in detail the relationship between strain, hydrogen solubility, and cohesive strength.

We present the results of ab-initio studies of H segregation in Fe single crystal {001} and {111} cleavage planes, as well as at a $\Sigma5$ symmetrical tilt grain boundary. We determine the solution energy as a function of tractions normal to the interface for different loading and relaxation schemes. While the chosen method clearly affects the quantitative results, the qualitative findings are the same: In relaxed as well as strained microstructures, H tends to accumulate at the grain boundary. While it reduces the surface energies, and hence the work of separation, there is no significant impact of H on the transgranular or intergranular fracture stress.

MM 33.3 Wed 10:45 IFW A

Solute - hydrogen interactions at Al grain boundaries: A first principle study — •Poulami Chakraborty, Tilmann Hickel, Baptiste Gault, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH

The deleterious effect of hydrogen on the mechanical properties of metallic alloys is known to reducestrongly limits the applicability of high strength metallic materials. Therefore, the characterization and simulation of hydrogen in such alloys is decisive. In this work, the interaction of hydrogen with GBs in aluminium in terms of decohesion effect has been investigated by means of density functional theory simulations. Two distinct types of GBs have been considered: the $\Sigma11(113)$ [011] with a close-packed interface structure and the $\Sigma5(210)$ [001] with a more open interface structure. We first identify the potential interstitial sites of H adsorption at GBs and then the mechanisms governing the H segregation energetics. A thermodynamic assessment of the impact of solutes onto H chemisorption in the interfacial vicinity is provided by performing a high-throughput analysis for potential alloying candidates. The identified trends of the solute-H interactions are comparable in the two representative cases studied, which motivated us to extend the work towards a more generalized approach.

MM 33.4 Wed 11:00 IFW A

Niobium Hydrogen Thin Films: Mechanical Stress, Interface Coherency and Phase Equilibria — •Stefan Wagner[1], Philipp Klose[1], Vladimir Burlaka[2], Kai Nörthemann[2], Magnus Hamm[2], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Göttingen University, Institute of Applied Materials, Göttingen, Germany

Metal-hydrogen systems offer grand opportunities for studies on fundamental aspects of alloy thermodynamics and kinetics. When the system size is reduced to the nanoscale, interface effects related to microstructural defects as well as mechanical stress affect the systems' properties [1]. In thin films the lattice expansion linked to hydrogen absorption is hindered by the substrate. Resulting stresses are usually compensated by plastic deformation, lowering the film's coherency state. Here we show for the model case of niobium-hydrogen (Nb-H) thin films on sapphire substrates that plastic deformation is suppressed below critical values of film thickness. This yields ultra-high stresses of up to -10 GPa, changing the film's phase stabilities, phase diagrams as well as the phases' nucleation and growth dynamics. [1] S. Wagner et al., Chem. Phys. Chem. 20 (2019) 1890.

MM 33.5 Wed 11:15 IFW A

ETEM studies on hydride precipitation and growth in Mg films — Magnus Hamm[1], Marian David Bongers[1], Vladimir Roddatis[1], Stefan Dietrich[2], Karl-Heinz Lang[2], and •Astrid Pundt[2] — [1]Göttingen University, Institute of Materials Physics (IMP), Göttingen, Germany — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Understanding solute-induced phase transformations is crucial in a variety of research fields such as catalysis, memory switching or energy storage. We present solute-induced phase transformations studied on the model system magnesium-hydrogen (MgH) which provides high lattice expansion during the phase transformation. In situ precipitation and growth of MgH2 is studied in an environmental transmission electron microscope (ETEM), combining electron energy loss spectroscopy (EELS) and various imaging techniques. We observe that the Mg-hydride (MgH2) formation proceeds through the formation of nanocrystals that are separated by low-angle grain boundaries. We attribute this microstructural change to large strains and stresses between the matrix and the MgH2 created during the transformation. [1] M. Hamm et al., Int. J. Hydr. Energy 44 (2019) 32112.

MM 34: Computational Materials Modelling - Matter-Particle Interaction

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

MM 34.1 Wed 10:15 IFW D

Structural evolution in a heavily irradiated BCC metal. — •Peter Derlet[1] and Sergei Dudarev[2] — [1]Condensed Matter Theory Group, Paul Scherrer Institute, Switzerland — [2]Department of Physics and Thomas Young Centre, Imperial College London, United Kingdom

Using atomistic simulations and a simplified and computationally highly efficient defect-creation protocol, we study the micro-structure emerging under high-dosage neutron and ion irradiation conditions. The so-called Creation Relaxation Algorithm (CRA) simulations exhibit the gradual transition from isolated defects to a micro-structure characterized by an extended dislocation network and a population of vacancy and interstitials. The corresponding internal stress/strain structure characterizes a spatially correlated and multi-scale potential energy-landscape whose material descriptors remain largely insensitive to further irradiation exposure. With full atomic resolution, the CRA rapidly produces a complex microstructure with strong experimental analogues in BCC materials experiencing doses relevant for the ITER fusion reactor project. Examples are given for both BCC Fe and W.

MM 34.2 Wed 10:30 IFW D

Post-ionization dynamics in proton-irradiated ice — •Daniel Muñoz-Santiburcio — CIC nanoGUNE, San Sebastián, Spain

Ion irradiation of water systems is receiving an increasing attention due to many important applications. In the case of liquid ice the main interests are the radiation damage of biological tissues and radiation treatment of tumors, while for water ice the interest concerns astrophysical/chemical processes taking place in interstellar dust, comets, asteroids and satellites.

Here I will show, in a first step, how it is possible to use the results of Ehrenfest MD simulations of the irradiation of ice with highly energetic protons to define plausible single- and double-ionized ice configurations; and in a second step, how these can be propagated via remarkably challenging ab initio MD simulations in order to observe different chemical reactions: *i*) the ultrafast conversion of the water cation H_2O^+ into the hydroxy radical $HO^\cdot$ plus the solvated H^+ which undergoes fast Grotthuss diffusion, and *ii*) the formation of H_2O_2 after the fragmentation of two neighboring H_2O^+.

MM 34.3 Wed 10:45 IFW D

Improved Stopping in the Binary Collision Approximation — •Alrik Stegmaier and Hans Hofsäss — 2. Physikalisches Institut, Universität Göttingen

Stopping of ions in materials is an important process in implantation physics, radiation safety, nuclear medicine, sputtering, proton beam writing and many more. As such, precise simulations of stopping are required, where typically a balance between accuracy and speed of the simulation is struck.

Due to the simplicity and relative accuracy, the binary collision approximation (BCA) is one of the most important models used for stopping today. In BCA stopping is treated as a series two body collisions.

Here we present an improved binary collision approximation model for ion stopping that is based on velocity dependent interatomic potentials. Both a new model for stopping of ions in an inhomogeneous electron gas and an approximate bond breaking/relaxation model for electronic stopping allow predictions over a large projectile velocity range and target structure.

The free parameters of the model are almost entirely constrained by density functional theory simulations and the properties of the (in-)homogeneous electron gas.

MM 34.4 Wed 11:00 IFW D

Quantum mechanical modelling of light-matter interactions — •Mark Kamper Svendsen and Kristian Sommer Thygesen — Technical University of Denmark, Kgs. Lyngby, Denmark

First-principles calculations based on density functional theory (DFT) have been pivotal for our understanding of the chemical, thermodynamic, and electronic properties of materials close to their ground state. However, when it comes to interaction with light such calculations are challenged in two important ways: First, the description of the electronic excited states is much more involved than the description of the ground state. In particular, collective excited states such as excitons or plasmons are challenging and not well described by standard DFT. Secondly, the light field is usually treated classically, and the quantum description is retained only for the electrons. This approximation can be justified in situations where the photon number is very large. However, in cases where the photon number is low and the field amplitude large, e.g. in cavities or near plasmonic structures, the quantum nature of the light field cannot be ignored.

We present a fully quantum mechanical model of the coupling between confined optical modes such as graphene plasmons and transitions in solid state systems. The model uses existing ab-inito methods to calculate the material properties and then uses those as input for accurate models of the light-matter interaction based on Macroscopic quantum electrodynamics.

MM 35: Topical Session: Data Driven Materials Science - Descriptors (joint session MM/CPP)

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

MM 35.1 Wed 11:45 BAR 205

Evaluating representations of atomistic systems for machine learning — •Marcel Langer[1] and Matthias Rupp[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Citrine Informatics, Redwood City, CA, USA

Interpolating between computationally expensive first-principles calculations with fast machine-learning surrogate models increases the feasible scope of exploration when a large space of potentially similar structures is sampled, for instance in the search for novel materials or the exploration of phase diagrams.

The choice of representation of the atomistic systems under consideration is important for the accuracy of such surrogate models. We present a rigorous empirical comparison of the Many-Body Tensor Representation [1], Smooth Overlaps of Atomic Positions [2], and Symmetry Functions [3] for energy predictions of molecules and materials. In this, we control for data distribution, hyper-parameter optimization, and regression method. We also investigate the relationship between predictive performance and computational cost, and discuss how to assess predictions beyond mean errors, which cannot fully describe model behaviour in practice. [4,5]

[1] H. Huo and M. Rupp, *arXiv*, 1704.06439 (2017)
[2] A. Bartók, R. Kondor., G. Csányi, *Phys. Rev. B* **87**, 184115 (2013)
[3] J. Behler, *J. Chem. Phys.* **134**, 074106 (2011)
[4] C. Sutton *et al.*, *ChemRxiv*, 9778670 (2019)
[5] Z. del Rosario *et al.*, *arXiv*, 1911.03224 (2019)

MM 35.2 Wed 12:00 BAR 205

Information-theory-driven identification of compact descriptors for accurate machine-learning predictions — •Benjamin Regler, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Machine learning (ML) is useful for predicting materials behavior by relating physical and chemical properties (features) of known materials to the property of interest (target). Aiming at a rational, unbiased, and data-driven identification of relevant features, we use a combination of statistical and information-theoretical techniques to identify the subset of features that unequivocally represent each material in the data set and contribute most to predicting the target property. The novelty and power of our approach is that it does not assume any specific functional form of the “features → target” relationship. Based on the concept of cumulative mutual information, our framework assigns quantitative scores for the “strength” of the feature’s contributions, ranks the features by their scores, and selects the most contributing features to be relevant prior to ensuing data analysis. The scoring and selection algorithm is then supplemented by a purely ML procedure built on the selected and compact feature subset. We identify compact feature subsets for predicting (i) the ground-state crystal-structure of octet-binary compound semiconductors and (ii) elastic properties of inorganic crystalline compounds. In each case, we show that only a few features are actually required to obtain accurate predictions, thereby reducing the complexity of the ML model and sensitivity to the availability of materials data.

MM 35.3 Wed 12:15 BAR 205

Size-Extensive Molecular Machine Learning with Global Descriptors — •Johannes Margraf[1], Hyunwook Jung[2], Sina Stocker[1], Christian Kunkel[1], and Karsten Reuter[1] — [1]Technical University Munich, Germany — [2]Yonsei University, South Korea

Machine learning (ML) models are increasingly used to predict molecular properties in a high-throughput setting at a much lower computational cost than conventional electronic structure calculations. Such ML models require descriptors that encode the molecular structure in a vector. These descriptors are generally designed to respect the symmetries and invariances of the target property. However, size-extensivity is usually not guaranteed for so-called global descriptors. In this contribution, we show how extensivity can be build into ML models with global descriptors such as the Many-Body Tensor Representation. Properties of extensive and non-extensive models for the atomization energy are systematically explored by training on small molecules and testing on small, medium and large molecules. Our results show that the non-extensive model is only useful in the size-range of its training set, whereas the extensive models provide reasonable predictions across large size differences. Remaining sources of error for the extensive models are discussed.

MM 35.4 Wed 12:30 BAR 205

Hierarchical SISSO: predicting complex materials properties building on simpler ones — •Lucas Foppa[1], Sergey V. Levchenko[2,1], Matthias Scheffler[1], and Luca M. Ghiringhelli[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Skolkovo Institute of Science and Technology, Moscow, RU

Symbolic regression is a promising tool to identify analytical models (descriptors) for predicting materials properties that are otherwise accessed via rather expensive *ab initio* calculations. In this context, the sure-independence screening and sparsifying operator (SISSO),[1] which combines the systematic generation of large feature spaces with compressed sensing, has been successfully applied, e.g., to the prediction of the (meta)stability of binary systems and perovskites from atomic properties only. However, if the relationship between the features and the target property is too complex, the descriptor search can become very inefficient. Here, we tackle this issue via a hierarchical approach: features that are easily computed (e.g., atomic properties) are used for predicting simple properties (e.g., lattice constant) and the resulting descriptors are in turn used as candidate features for modeling more complex properties (e.g., bulk modulus, position of band centers or band gaps). We demonstrate the hierarchical approach by analyzing a dataset of >700 cubic simple ($AB\mathrm{O}_3$) and double ($A_2BB'\mathrm{O}_6$) perovskites for predicting mechanical and electronic properties. The learned models require only atomic features as inputs and are therefore suitable for high-throughput screening of such materials.

[1] R. Ouyang, *et al.*, *Phys. Rev. Mater.* **2**, 083802 (2018).

MM 35.5 Wed 12:45 BAR 205

Similarity descriptors for data-driven materials science — •Martin Kuban, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Learning from materials data is a topic of increasing importance in materials science. This task is supported by the availability of data through large online databases, like NOMAD [1]. For the application of artificial-intelligence (AI) methodology, materials must be characterized by a set of features that together build up *descriptors*. The success of AI tasks depends heavily on the quality of these descriptors, since they must contain all relevant information to map the input data onto the target property. Recent advances in the development of high-quality descriptors have allowed for both accurate predictions of material properties as well as highly interpretable models [2]. In this work, we develop a new type of descriptors based on the similarity of materials. To achieve this goal, we use both existing and newly developed descriptors to establish metrics that serve as quantitative similarity measures. These measures are combined into "similarity descriptors", which are then used for the construction of AI models. The performance of these models is optimized with respect to their predictive power. We demonstrate the applicability of our approach by predicting target properties for different classes of materials, including oxides and 2D systems.

[1] C. Draxl and M. Scheffler, MRS Bulletin, 43, 676, (2018).
[2] L. Ghiringhelli *et al.*, PRL, 114, 105503, (2015).

MM 35.6 Wed 13:00 BAR 205

Machine-learning descriptors with domain knowledge of the interatomic bond — •Thomas Hammerschmidt, Jan Jenke, Aparna P.A. Subramanyam, Jörg Kossmann, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The performance of machine-learning depends critically on the quality of the descriptors. In the case of learning atomic-scale properties, like formation energies obtained from density-functional theory (DFT) calculations, the descriptors typically measure the atomistic geometry and the distribution of chemical elements. Here, we construct descriptors that additionally include prior knowledge of the interatomic bond from a hierarchy of coarse-grained electronic-structure methods. In particular, we use tight-binding (TB) and analytic bond-order potentials (BOPs) that are derived from a second-order expansion of DFT. We demonstrate that a recursive solution of the TB problem and the closely related moments of the electronic density-of-states at the BOP level establish a smooth structure-energy relation. This first level of domain knowledge of the interatomic bond shows highly descriptive power in machine-learning applications already with simple, qualitative TB models. As second level of domain knowledge we include the bond chemistry in terms of bond-specific TB Hamiltonians that are obtained from downfolding the DFT eigenspectrum of molecular dimers. In the third level of domain knowledge we include the role of the valence electrons by determining non-selfconsistent bond energies with the bond-specific TB Hamiltonians.

MM 36: Topical Session: Interface-dominated phenomena - Theoretical Approaches

Time: Wednesday 11:45–13:00 Location: IFW A

Topical Talk MM 36.1 Wed 11:45 IFW A

Computational methods for grain boundary engineering — Daniel Scheiber, Vsevolod Razumovskiy und •Lorenz Romaner — Materials Center Leoben Forschung GmbH, Leoben, Austria.

Segregation of solute elements to grain boundaries plays an important role for the physical properties of many technologically relevant materials. For example, it can induce intergranular embrittlement in steels, copper, nickel-based alloys or refractory metals. Furthermore, also nanocrystalline stability, grain growth, phase transformations and electrical properties can be steered via segregations. Controlling such phenomena provides a lever for developing materials with superior or targeted properties.

In this talk we will present our recent activities regarding grain boundary engineering. This involves the development of computational methodologies providing direct coupling of atomistic grain boundary simulations with thermo-kinetic modeling. With such approaches, we describe the evolution of grain boundary chemistry during heat treatment, analyze depletion zones next to grain boundaries and explore the relationship with precipitation kinetics. The methods are applied to steels and refractory metals to show how chemical composition, grain size and heat treatment can be designed to reduce the propensity for intergranular cracking. As a last point we present the development of our software tool SEGROcalc and conclude with an outlook on challenges for future segregation modeling.

MM 36.2 Wed 12:15 IFW A

Towards large-scale atomistic calculations with quantum-mechanical accuracy: the QM/MM route — •Gehringer Dominik[1], Liam Huber[2], Jörg Neugebauer[2], and David Holec[1] — [1]Department Materials Science, Montanuniversität Leoben, Franz-Josef-Straße 18, 8700 Leoben — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf

Although ab-initio methods such as Density Functional Theory (DFT) provide a powerful tool to investigate materials science problems, they are also a limiting factor in terms of tractable system sizes, especially when one moves on to extended defects (interfaces, grain boundaries, dislocations). In constrast to DFT molecular dynamics (MD) is also well suited to properly describe temperature and mechanical properties, since simulations can handle thousands of atoms needed for describing extended defects. On the other hand, since in MD simulations do not consider the electronic structure but rather rely on interatomic potentials, the accessible chemistry is restricted by the availability of those. This is a limiting factor for e.g. segregation studies.

In the present contribution we will describe our developments for linking quantum mechanical calculations with molecular mechanics. While MM is applied to matrix regions, QM is used to treat chemical impurities and extended defects such as interfaces for which interatomic potentials are not available. After introducing the methodology and its implementation within the pyiron framework, we will show an example of linking LAMMPS and VASP calculations on an example of segregation to phase boundaries in γ/α_2 structured TiAl alloys.

MM 36.3 Wed 12:30 IFW A

Characterization of the stability of metal/metal interfaces by atomistic simulations — •Daniel F. Urban[1], Oskar Till[2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

The reliable prediction of the adhesion and mechanical stability of interfaces between two metal phases from density functional theory (DFT) calculations remains a challenge. One possible approach to systematically address this issue is an idealized cleavage simulation analysed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. Another approach is the study of the gamma surface, i.e. the generalized stacking fault energy, as function of lateral displacement, which yields information on the critical resolved shear stress of dislocation motion.

Here we study a variety of coherent interfaces between fcc and hcp metals in terms of the above mentioned methods. We analyze the interface energy in terms of coupled tensile and shear displacements which include the effect of the tension softening of the interface. Furthermore, the influence of an additional lateral mechanical strain on the two phases, as often present in experimentally grown thin layers, is examined.

MM 36.4 Wed 12:45 IFW A

Comparative atomistic-continuum modeling and experimental characterization of dislocation-solute interaction in binary alloys — •Jaber R. Mianroodi[1,2], Pratheek Shanthraj[2,3], Xuyang Zhou[2], Gregory B. Thompson[4], and Bob Svendsen[1,2] — [1]RWTH Aachen University, Aachen, Germany — [2]Max-Planck-Institut fur Eisenforschung, Dusseldorf, Germany — [3]The University of Manchester, Manchester, UK — [4]The University of Alabama, Tuscaloosa, USA

The purpose of the current work is a comparative modeling and experimental investigation of the interaction between defects and chemistry in metallic alloy systems at the nanoscopic scale. On the modeling side, three approaches are employed and compared. These include (i) hybrid Monte-Carlo molecular dynamics (e.g., [1]), (ii) diffusive molecular dynamics (e.g., [2]), and (iii) atomistic phase-field chemomechanics (e.g., [3]). All these are energy-based approaches. In the first two, the energy is determined by an interatomic potential. For (quantitative) comparability, the same potential is used to calibrate the phase-field energy model. In the current work, these three methods are applied to the modeling of solute segregation to dislocations in the binary system Pt-Au. Corresponding simulation results are compared with analogous experimental results from atom probe tomography and precession electron diffraction. Among others, these include in particular results on solute segregation to the dislocation core as well as on maximum segregation to dislocations at different bulk compositions.

MM 37: Materials for Energy Storage and Conversion - Structure of Battery Materials

Time: Wednesday 11:45–13:00 Location: IFW D

MM 37.1 Wed 11:45 IFW D

Analytical TEM studies of $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$, $LiCoO_2$, and Si electrodes for Li-ion batteries — •Ardavan Makvandi[1], Martin Peterlechner[1], Simone Casino[2], Tobias Gallasch[2], Martin Winter[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]MEET Battery Research Center, University of Münster, Münster, Germany

The modification of state-of-the-art electrodes by nanostructured coatings is one approach to optimize crucial parameters for applications, such as the electronic conductivity or mechanical stability. In general, interfaces (e.g. active material/coating; electrode surface/electrolyte) determine the local Li-ion transport kinetics and finally the electrochemical performance in terms of cycling stability or capacity retention. Therefore, it is necessary to study the structure and chemistry of electrodes and electrode/electrolyte interfaces. In this work, the structure and chemistry of the bulk and surface regions of $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC-622), $LiCoO_2$ (LCO), and Si electrodes after cycling are studied using transmission electron microscopy (TEM). In the case of NMC-622 and LCO electrodes, the effect of an Al doped ZnO-coating layer on the stability of the surface upon cycling is studied. Moreover, in the case of a Si electrode, the effect of a carbon-coating layer on the strain evolution caused by the volume expansion during cycling is studied.

MM 37.2 Wed 12:00 IFW D

Creating an NCM thin film cathode model system for the interface analysis of liquid electrolyte batteries — •Hendrik Hemmelmann[1,2], Julius K. Dinter[1,2], Juri E. Becker[1,2], Angelika Polity[2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Justus-Liebig-University Giessen, Germany — [2]I. Physikalisches Institut, Justus-Liebig-University Giessen, Germany

Coating the active cathode material (CAM) with a chemically inactive layer can significantly improve the performance of lithium ion batteries (LIBs). However, the reason for the beneficial effect of the coating is lacking a deeper understanding. Here, we present the preparation of lithium nickel cobalt manganese layered oxide (NCM) thin films, which were subsequently coated with Al2O3 of different thicknesses using atomic layer deposition (ALD). Such thin films are ideal model systems to characterize the interface properties using surface-sensitive techniques. To investigate the influence of the coating, electrochemical measurements were performed using metallic Li as anode and the interface properties were characterized using XRD, SEM, AFM, Raman and XPS.

MM 37.3 Wed 12:15 IFW D

Highly stable and highly conductive LiCoPO4 olivine-based thin film 5V cathode material. — •Gennady Cherkashinin[1], Robert Eilhardt[1], Silvia Nappini[2], Igor Píš[2], Federica Bondino[2], Simone dal Zilio[2], Elena Magnano[2], Matteo Cococcioni[3], and Lambert Alff[1] — [1]Technische Universität Darmstadt, Germany — [2]IOM CNR Laboratorio TASC, Basovizza, TS, Italy — [3]Physics Department, University of Pavia, Italy

Recently, we have discovered high electronic conductivity of the LiCoPO4 olivine 5V cathode thin film material tailored with LiCo2P3O10. The crystal structure of the compound remains stable even if all Li-ions leave the olivine structure, which corresponds to ~5.1V vs. Li+/Li. Here we explore the intrinsic stability of the novel thin film cathode material and the stability of cathode/electrolyte interface upon the charging/discharging potential in the 3.0-5.1V range. We apply the comprehensive in-situ electron spectroscopy approach (XPS and XAS) combined with first principle calculations to study the evolution of the oxidation and valence states, the Co3d-O2p hybridization, the work function, the density of occupied and unoccupied states near the Fermi level, the chemical composition, etc. as a function of the Li-content. We show that the electronic structure/properties of the compound are fully reversible; LiCo2P3O10 stabilizes the olivine structure in its fully delithiated state. First-principles simulations predict ~5.2V redox for LiCo2P3O10. Thus, higher energy density via the involvement of LiCo2P3O10 into the redox reaction is possible. A reason of enhanced conductivity at atomic level is analyzed.

MM 37.4 Wed 12:30 IFW D

First-principles investigation of a LISICON-to-LGPS phase transition in $Li_{10}GeP_2O_{12}$ — •Giuliana Materzanini and Nicola Marzari — Theory and Simulations of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Using ab-initio molecular dynamics, we have recently reported a remarkably high Li-ion conductivity ($\sigma \simeq 10^{-3}$S/cm at 25°C, $E_a = 0.21$ eV) for the oxide analogue of $Li_{10}GeP_2S_{12}$ (LGPS, tetragonal $P4_2$/nmc). Though not being reported in the experimental literature so far, this system possesses the same density and stoichiometry of the LISICON $Li_{3.33}Ge_{0.33}P_{0.66}O_4$ (orthorhombic Pnma), that oppositely shows low conductivity ($\sigma \simeq 10^{-6}$S/cm at 25°C, $E_a = 0.54$

eV). Aim of this work is shedding light on a possible phase transition from the existing orthorhombic phase to a tetragonal phase of $Li_{10}GeP_2O_{12}$ (LGPO). We use variable-cell (NPT) Car-Parrinello molecular dynamics (CP package of the QUANTUM ESPRESSO distribution) at 600K, 1200K an 1500K. Simulations are conducted starting from both the tetragonal ideal LGPS structure (t-LGPO) and the existing orthorhombic structure (o-LGPO). Although t-LGPO has higher enthalpy than o-LGPO at all temperatures, at 1200K o-LGPO undergoes phase transitions, possibly driven by the higher entropy and Li-ion conductivity of the phases formed during the dynamics. Structural similarities with t-LGPO of these phases are discussed, and their conductivities at 600K assessed through NPT and NVT simulations.

MM 37.5 Wed 12:45 IFW D

Graded electrodes for lithium-ion batteries — •Chuan Cheng[1], Ross Drummond[2], Stephen Duncan[2], and Patrick Grant[3] — [1]Warwick Manufacturing Group (WMG), University of Warwick, Coventry CV4 7AL, UK — [2]Department of Engineering Science, University of Oxford, Oxford OX1 3PJ, UK. — [3]Department of Materials, University of Oxford, Oxford OX1 3PH, UK.

Homogeneous electrode structures used in conventional Li-ion batteries (LIB) lead to inhomogeneous active material utilization and gradients of overpotential and Li-ion concentration at the cell-scale, which are detrimental for both capacity retention at high charge-discharge rates and for battery lifetime. To account for these gradients, we demonstrate that heterogenous electrode structures with engineered gradients in material distribution can improve LIB C-rate and long-term cycling performance when compared with conventional uniform electrodes in full-cell and half-cell LIBs. The improved performance of graded electrodes is shown to derive from a lower charge transfer resistance and reduced polarization at high C-rates, which suggests a more spatially homogeneous distribution of over-potential and hindering of the side reaction-induced battery degradation during long-term cycling.

References

[1] C. Cheng, R. Drummond, S. R. Duncan, and P. S. Grant, J. Power Sources 413, 59 (2019).

[2] C. Cheng, R. Drummond, S. R. Duncan, and P. S. Grant, J. Power Sources, In Press. https://doi.org/10.1016/j.jpowsour.2019.227376

MM 38: Invited talk Körner

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

Invited Talk MM 38.1 Wed 15:00 BAR 205

Single Crystals of Alloys by Additive Manufacturing — •Carolin Körner, Markus Ramsperger, Julian Pistor, Johannes Köpf, and Matthias Markl — Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl WTM, Martensstr. 5, 91058 Erlangen

In materials science, single crystals are used for high strength materials with high creep resistance such as turbine blades from nickel-base superalloys. The fabrication techniques used to produce single crystals involve highly controlled and therefore relatively slow crystallization. For turbine blades, the Bridgman technique, i.e. investment casting combined with direction solidification, is the standard. The single crystal either develops starting from a single crystalline seed or by a geometric grain selection process. Microstructure evolution is determined by the solidification conditions resulting in a dendrite arm spacing of several hundreds of microns. This contribution shows how single crystals from nickel-base superalloys develop without seed during layer by layer metal additive manufacturing in the powder bed. These AM single crystals develop under rapid and directional solidification conditions with solidification microstructures two orders of magnitude finer than in the conventional Bridgman process. The basis mechanisms leading to the single crystal and the implications on the resulting mechanical properties are discussed.

MM 39: Computational Materials Modelling - Alloys I

Time: Wednesday 15:45–17:00 Location: BAR 205

MM 39.1 Wed 15:45 BAR 205

Atomistic spin dynamics coupled with *ab initio* molecular dynamics simulations of Fe in the paramagnetic state — •Davide Gambino and Björn Alling — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden

Accurate investigation of magnetic materials at finite temperatures with first principles methods is a formidable task that requires inclusion of magnetic and vibrational effects on a similar footing in order to account for their interplay. An approach that allows to investigate the coupling of these different degrees of freedom is the atomistic spin dynamics - *ab initio* molecular dynamics (ASD-AIMD) method [Stockem *et al.*, *Physical Review Letters* 121, 125902 (2018)], in which an AIMD and an ASD simulations are run in parallel communicating to each other atomic positions (which affect exchange interactions) and magnetic moments directions.

While the method was initially tested on CrN, a semiconducting system with well localized magnetic moments, in this work we perform an ASD-AIMD investigation of Fe in the paramagnetic state, close to its Curie temperature. Since Fe is a ferromagnetic metal, it is relevant to investigate also the contribution of longitudinal spin fluctuations (LSF) to the thermodynamics of the system. LSF are here included through a mean-field term derived from a semiclassical model. The present results pave the way for free-energy calculations in magnetic materials by means of *ab initio* methods.

MM 39.2 Wed 16:00 BAR 205

Disorder driven stability in Co-based Heusler compounds — •Vitaliy Romaka, Ahmad Omar, Sabine Wurmehl, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

Co-based Heusler compounds are known as promising half-metallic magnetic materials. However, their magnetic properties are affected by various factors, such as anti-site disorder, vacancies, and thermodynamic instability. Particularly in the case of systems that, in addition to Co, contain other $3d$ metals, for example Fe and/or Cr, the structural and thermodynamic issues are not very well understood. In order to shed light on the effects of structural disorder and off-stoichiometry in Co-based Heusler compounds, a section of the thermodynamic phase diagram for the quaternary Co-Cr-Fe-Al system was investigated by means of *ab initio* calculations. In the case of $Co_2Cr_{1-x}Fe_xAl$ solid solution, with energetically favorable $B2$-type structure, the shape of thermodynamic potential is quite similar to what is expected in the case of spinodal decomposition of the solid solution and is further characterized by two local minima at $x \sim 0.3$ and 0.7, which describe the binodal region. Thermodynamic instability is also observed in the $CoCr_{1-x}Al_x$ and $CoFe_{1-x}Al_x$ solid solutions. Despite the fact that the quaternary composition $Co_2Cr_{0.5}Fe_{0.5}Al$ is electronically equivalent to the thermodynamically stable Co_2MnAl phase, DFT modeling shows that the composition with higher Al content ($\sim Co_2Cr_{0.3}Fe_{0.5}Al_{1.2}$) is energetically more stable, especially at high temperatures which is consistent with the experimental data.

MM 39.3 Wed 16:15 BAR 205

Investigating anharmonicity in BCCs: from unaries to HEAs — •Prashanth Srinivasan[1], Blazej Grabowski[2], Alexander Shapeev[3], Jörg Neugebauer[4], and Fritz Körmann[1,4] — [1]TU Delft — [2]University of Stuttgart — [3]Skolkovo Institute of Science and Technology — [4]MPIE Dusseldorf

Anharmonicity is a major contributor to the vibrational free energy of metals, especially at high temperatures. It has been shown for an extensive set of FCC unaries that the anharmonic Gibbs energy contribution is positive and increases with temperature [Glensk et al., 2015].

Unlike in FCC metals, empirical works [Wallace, 2002] suggest some BCC metals to have negative anharmonic contributions to the total free energy. Computational first-principles studies beyond quasiharmonicity are, however, scarce owing to the expensiveness of such calculations. Recent advances combining efficient thermodynamic sampling schemes and machine-learnt moment tensor potential [Grabowski et al., 2019] allow for an efficient yet numerically accurate vibrational free energies determination including anharmonicity. Using this, anharmonic free energies for a set of BCC metals from unaries up to five-component multicomponent alloys are calculated and discussed. As for the unaries, the anharmonicities of different sets of alloys can show both positive as well as negative anharmonic contributions depending on alloy composition.

MM 39.4 Wed 16:30 BAR 205

Ab initio study of carbon and nitrogen interstitials in CoCrNi high entropy alloy — •Martin Zelený[1], Igor Moravčík[1], Martin Friák[2], and Ivo Dlouhý[1,2] — [1]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

Twinning-induced plasticity of CoCrNi medium entropy alloy (MEA) is responsible for its extraordinary strength-ductility-toughness combination. In present work we used density functional theory to investigate the effect of interstitial nitrogen and carbon atoms on phase stability, stacking-fault energy and magnetic properties. To describe alloys with chemical disorder as MEAs we employed directionally-optimized supercell-based quasirandom structures. We found that both elements stabilize fcc structure with respect to hcp structure which results in lower probability to create a stacking fault. On the other hand, the effect on magnetic properties is negligible.

MM 39.5 Wed 16:45 BAR 205

Magnetic ordering in Mo-based HEA — •Jakub Šebesta[1,2], Karel Carva[2], and Dominik Legut[1] — [1]Nanotechnology Centre & IT4Innovation, VŠB-TU Ostrava, 17.listopadu 2172/15 708 00 Ostrava-Poruba, Czech Republic — [2]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5 121 16 Praha 2, Czech Republic

The multiprincipal element alloys stand for promising materials with the wide range of possible application *e.g.* in the mechanical engineering. Ones of the most known representatives are the high entropy alloys (HEA). They benefit from composing of several components, originally five (but also less), which leads to the high temperature stabilization, higher creep and oxidation resistance, improved ductility and mechanical strengths. In composition of many of them a 3d magnetic element like Cr, Mn, Fe, Co, and Ni appears. Naturally the question arises, what is the influence of such element on magnetic ordering, on the alloy stability, magnetic order and how it alter all above mentioned properties. Therefore, in this study we discuss the enhancement of the magnetic order given by a Mo substitution in the well known Cantor alloy based on ab-initio calculations employing the TB-LMTO-ASA method. This allows us to treat a disorder efficiently within the framework of the CPA. The influence of the crystal structure and the position of the Mo-substitution on the stability and the magnetic behavior is shown. The evaluation of the strength of the magnetic exchange interactions lead to the determination of T_{C}.

MM 40: Topical Session: Interface-dominated phenomena - Solutes at Interfaces I

Time: Wednesday 15:45–17:00 Location: IFW A

Topical Talk MM 40.1 Wed 15:45 IFW A

Using interfaces to move solute atoms and using moved atoms to stop interfaces in steels — •Sybrand van der Zwaag — TU Delft, Delft, the Netherlands

Diffusional phase transformations in steels can involve the partitioning of substitutional alloying elements at the moving austenite-ferrite interface. Under normal isochronal or isothermal annealing conditions the local solute enrichment is spatially coupled to (one side of) the interface at all times. However, in the cyclic partial phase transformation approach, the direction of the moving interface is reverted periodically and the enriched region and the crystallographic interface separate due to a difference in mobility. Hence, reversing the direction of the interface allows for the creation of narrow (nm wide) regions with a higher concentration of substitutional alloying elements within the crystallographically unaffected parent austenitic matrix. Multiple passes towards the enriched rim left behind in the first partial transformation cycle will increase the local enrichment even further. The enriched rim manifests itself as a (chemical) barrier and can block the interface upon final cooling for as much as 150 K. The interface motion and blocking effects are analysed using dilatometry, laser scanning confocal microscopy and Transmission Electron Microscopy.

The chemical boundary engineering (CBE) concept has then been used to create steels in which the sharp boundaries of enriched domains locally halt the advancing martensitic phase fronts, resulting in a nanostructured multiphase steel with exceptional mechanical properties.

MM 40.2 Wed 16:15 IFW A

Atomic scale structure and segregation behavior at $\Sigma 5$ tilt grain boundaries in bcc iron — •Ali Ahmadian, Xuyang Zhou, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries (GBs) are two-dimensional defects, which determine the mechanical as well as physical properties of polycrystalline materials. Segregation of impurities, such as phosphorous, to GBs can reduce their cohesive strength and with this lead to embrittlement of a material. By introducing other impurities such as carbon, the segregation tendency of phosphorous can be suppressed. It is under debate whether boron has the same effect as carbon and how a co-segregation of both elements influences GB properties [1]. In this work, we investigated ferritic Fe-2wt%Al bicrystals grown by a modified Bridgeman technique. The global structure of the GB is characterized by electron backscatter diffraction, revealing a symmetric $\Sigma 5$ [001] (310) tilt GB. Aberration-corrected scanning transmission electron microscopy experiments showed kite-type structural units as predicted by atomistic simulations by Scheiber et al. [2]. However, the atomic structure of the GB also contains other defects such as facets or steps, leading to different local reconstructions. In combination with atom probe tomography experiments, a clear segregation of both carbon and boron is observed, while aluminium is depleted at the boundary. The latter one is in contradiction to DFT calculations, where a clear segregation of aluminium was predicted. [1] C. M. Liu et al., Metall Trans A 23 (1992) [2] D. Scheiber et al., MODEL SIMUL MATER SC 24 (2016)

MM 40.3 Wed 16:30 IFW A

Correlative study of grain boundary segregation in nanocrystalline copper-nickel alloys — •Felix Fischer, Rüya Duran, and Guido Schmitz — Institute for Materials Science, University of Stuttgart, Germany

Nanocrystalline material properties are dominated by grain boundaries (GB). In nanocrystalline copper-nickel alloys, which have high corrosion resistance, thermal conductivity and fabricability, segregation of copper to GBs is energetically preferred and was previously quantified in simulations. In these simulations the values for excess segregation depend highly on grain boundary structure, therefor transmission electron backscatter diffraction (t-EBSD) and atom probe tomography (APT) measurements are carried out on prepared nanocrystalline tips.

t-EBSD allows an evaluation of the grain orientations and thus the GB types, while APT gives an atomically-resolved digital reconstruction of the measured tip. Combing these two methods, the segregation of copper to GBs can be correlated to the GB type, alloy concentration as well as the annealing temperature and furthermore compared to simulated segregations. By applying molecular dynamic simulations, additionally, the excess segregations of so far unevaluated GBs can be obtained and directly compared to experimental results.

The presentation will elucidate in detail the experimental procedure and shortly mention the used simulation methods from which the correlations of GB segregation to GB type, concentration and temperature are determined and also compared between theory and experiment.

MM 40.4 Wed 16:45 IFW A

The effect of grain boundary segregation on embrittlement: recent trends and open questions — Pavel Lejček[1] and •Mojmir Šob[2,3,4] — [1]Inst. Phys., Acad. Sci. Czech Rep., Prague — [2]Masaryk Univ., Fac. Sci., Dept. of Chem., Brno, Czech Rep. — [3]Inst. Phys. Mat., Acad. Sci. Czech Rep., Brno — [4]Central Europ. Inst. Technol., CEITEC MU, Masaryk Univ., Brno

To elucidate the effect of individual solutes on embrittlement of various base materials such as steels and nickel-base superalloys, grain boundary and surface segregation was extensively studied in many laboratories. Unfortunately, the values of the segregation energy of a solute at grain boundaries as well as at the surfaces obtained by various authors sometimes differ by more than one order of magnitude: such a difference is unacceptable as it cannot provide us with representative view on the problem of material temper embrittlement Here we summarize the available data on interfacial segregation and embrittlement of various solutes in nickel and bcc iron and critically discuss their reliability, assessing also limitations of individual approaches employed to determine the values of segregation and strengthening/embrittling energies. We demonstrate that theoretical approaches are limited by the size of the computational repeat cell used for the calculations of the segregation energy. On the other hand, the change in the grain boundary cohesion (strengthening/embrittling energy) may be obtained with a reasonable accuracy. For many impurities, there is lack of experimental segregation data. Therefore, many calculated results are theoretical predictions which may motivate future experimental work.

MM 41: Computational Materials Modelling - Solids and Molecules (joint session MM/CPP)

Time: Wednesday 15:45–17:00 Location: IFW B

MM 41.1 Wed 15:45 IFW B

Molecular Adsorption Potential Energy Surfaces and their Reproducibility — •Lukas Hörmann, Andreas Jeindl, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Molecular adsorption on surfaces depends on a range of mechanisms: covalent bonds, charge transfer and van-der-Waals (vdW) interactions shape the potential energy surface (PES), making the PES key to understanding molecule-substrate interfaces. Describing these interfaces with density functional theory requires a wise selection of the exchange correlation functional and vdW correction scheme. To explore the robustness of the PES with respect to the choice of method, we present a benchmark of common local, semi-local and non-local functionals in combination with various vdW corrections. We investigate these methods using perylenetetracarboxylic dianhydride (PTCDA) on Ag(111), one of the most frequently studied systems.

We use an in-house developed Gaussian process regression algorithm, which requires only about 50 DFT calculations as input to generate a PES with DFT accuracy. This allows a detailed analysis of the PES's features, such as positions and energies of minima and saddle points. Comparing the results from different exchange correlation functionals enables us to identify trends and differences between the approaches. Finally, we compare key features, such as local minima, with experimental data to determine a "quality seal" for the different functionals and vdW corrections.

MM 41.2 Wed 16:00 IFW B

The role of structural symmetry for proton tautomerization in aromatic molecules — •Antonios Raptakis[1,2], Alexander Croy[2], Rafael Gutierrez[2], Arezoo Dianat[2], and Gianaurelio Cuniberti[2] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Proton tautomerization is a prototype reaction and controllable on a single molecule level. In particular, studies of aromatic molecules, such as porphyrins and phthalocyanines, show the potential of use in molecular electronics, sensor devices and solar cells. Here, we simulate the reaction paths using well-tempered Metadynamics simulations, in molecular dynamic engine of DFTB+. We study the influence of symmetric and asymmetric functionalization on the tautomerization rates and metastable states of porphyrin and porphyrazine cores.

MM 41.3 Wed 16:15 IFW B

First-principles description of phase transitions in solids with rotating molecules and diffusing atoms — •Sergei Simak — IFM, Linköping University, Sweden

Solids with rotating molecules and diffusing atoms are examples of dynamically disordered phases of materials with great potential for applications, from fuel cells to optoelectronics. Description of thermodynamics of these materials is a challenge, as standard methods, like static phonon calculations fail due to the large displacements of atoms or the absence of well-defined equilibrium atomic positions. We briefly outline a method that offers a solution to the problem based on a stress-strain thermodynamic integration [1]. An example of lithium carbide, a fascinating material that combines strong covalent and weak ionic bonding resulting in a wide range of unusual properties, is considered [2]. The mechanism of its phase transition from the ground-state orthorhombic to the high-temperature cubic crystal, which is subject to both rotations of C-C dumbbells and Li self-diffusion, is revealed, and the thermodynamics is described.

[1] J. Klarbring and S. I. Simak, Phys. Rev. Lett. 121, 225702 (2018).
[2] S. Filippov, J. Klarbring, U. Häussermann, and S. I. Simak, Phys. Rev. Materials 3, 023602 (2019).

MM 41.4 Wed 16:30 IFW B

Development of a Neural Network Potential for Metal-Organic Frameworks — •Marius Herbold, Marco Eckhoff, and Jörg Behler — Georg-August Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

Metal-organic frameworks (MOFs) are crystalline porous materials with many applications in chemistry and materials science, from gas separation to heterogeneous catalysis. Computer simulations of chemical processes in MOFs are severely limited by the use of classical force fields (FFs), because most FFs are unable to describe bond formation and breaking. In principle, electronic structure methods, like density-functional theory (DFT), can overcome this problem, but often the required systems are too large for routine applications of DFT. Here a high-dimensional neural network potential (NNP) is presented for a series of MOFs, which combines the advantages of both worlds - the accuracy of first principle methods with the efficiency of simple empirical potentials. We demonstrate the possibility to obtain a reliable description of the potential-energy surface of bulk MOFs based on reference calculations of molecular fragments only.

MM 41.5 Wed 16:45 IFW B

Analysis of organic-inorganic thermal interfaces in Metal-Organic Frameworks — •Sandro Wieser[1], Tomas Kamencek[1], Rochus Schmid[2], Johannes Peter Dürholt[2], Natalia Bedoya Martínez[3], and Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Chair of Inorganic Chemistry 2, CMC Group, Ruhr-Universität Bochum, Germany — [3]Materials Center Leoben, Austria

Metal-Organic Frameworks (MOFs) represent a type of porous materials that show promising properties for many applications including gas-storage and catalysis, which in most of the cases rely on the effectiveness of dissipating heat. Due to the complex structure of these materials, an in depth understanding of how the fundamental structural characteristics of individual building blocks, as well as their interconnection, impact the system's properties is necessary. To that aim, we investigate isoreticular and tetragonal MOFs utilizing classical non-equilibrium molecular dynamics simulations. The interatomic interactions are described by specifically tailored MOF-FF potentials fitted to density-functional-theory reference data. From the obtained temperature profiles one can conclude that the factor primarily limiting thermal transport is a weak thermal coupling across the interface between the inorganic nodes and the organic linkers combined with a poor conduction within the nodes. We additionally investigate, how the thermal coupling across the heterointerface is impacted by parameters like the mass and extent of the individual components and the docking chemistry.

MM 42: Materials for Energy Storage and Conversion - Functional Materials

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

MM 42.1 Wed 15:45 IFW D

Charge carrier diffusion in $MgSc_2Se_4$ spinel structures — •Manuel Dillenz, Mohsen Sotoudeh, and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

New battery technologies have to meet a multitude of requirements in order to compete with Li-ion batteries, among them a sufficiently high ionic mobility both in the electrolyte and the electrodes. Materials that crystallize in the spinel structure represent promising materials that could meet this requirement. Here we present first-principles electronic structure calculations based on density functional theory (DFT) that have been performed to study the charge carrier diffusion in the $MgSc_2Se_4$ spinel structure. $MgSc_2Se_4$ exhibits very low diffusion barriers for Mg ion diffusion and is therefore a good candidate for solid electrolytes in Mg-ion batteries. In order to elucidate the factors determining the ion mobility we have also determined the diffusion barriers of other mono- and bivalent ions in this material and various other spinel structures in order to be able to derive chemical trends. These calculations show that the size and the charge of the ions influence the ion mobility. We will discuss further factors that could affect the ion mobility.

MM 42.2 Wed 16:00 IFW D

Defect Calculations to Explain Charge-Carrier Transition in Disordered Chalcogenides — •Valentin Evang[1], Johannes Reindl[2], Alexander Rochotzki[2], Matthias Wuttig[2,3], and Riccardo Mazzarello[1,3] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen — [2]I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen — [3]JARA-FIT, RWTH Aachen University, 52056 Aachen

Phase-change materials (PCMs) like GeSbTe and other chalcogenides promise to be key ingredients for future non-volatile memory thanks to their remarkable dynamic properties when switched between their crystalline and amorphous phases. Furthermore, they show features in atomic bonding, recently coined metavalent, that are incompatible with the well-known bonding types and could play an important role in the design of materials with specific phase-change properties.

For a related material, the disordered cubic phase of PbSbTe, experiments reveal a transition from n-type to p-type conduction as a response to annealing at high temperatures. During this process, only subtle changes in the crystal structure take place, pointing towards varying types of self-doping to cause the transition.

Here, we employ density functional theory to compute the formation energies of various possible defects in the disordered cubic and related phases of PbSbTe. It is found that, upon reducing the disorder on the lattice, the most favorable defect type changes in accordance with the observed n-to-p charge-carrier transition, representing a mechanism to tailor transport properties in PCMs by their level of disorder.

MM 42.3 Wed 16:15 IFW D

Understanding the charge trapping-detrapping in undoped- and carbon doped GaN — •Suchinder Sharma[1,2], Friederike Zimmermann[1], Jan Beyer[1], Eberhard Richter[3], and Johannes Heitmann[1] — [1]Institute of Applied Physics, Technical University Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz-Institute Freiberg for Resource Technology, 09599 Freiberg, Germany — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany

In the present contribution, we present our results on the thermoluminescence (TL) experiments on the GaN samples prepared by HVPE method, to understand the charge trapping-detrapping dynamics in the temperature range, 273-650 K. Interestingly, the undoped GaN sample showed a persistent luminescence (PersL) emission upon band-to-band and localized excitations (blue, green and red), which lasts for more than 9 h. Upon carbon doping, the PersL is quenched significantly, suggesting, that the population of defects responsible for the room temperature trapping-detrapping decreases with an increase in the carbon doping. Further, for low carbon containing sample, a new deep defect around 530 K is observed. The population of this defect further decreases for high carbon containing samples.

MM 42.4 Wed 16:30 IFW D

Electronic structure and core electron fingerprints of caesium-based antimonides for ultra-bright electron sources — Caterina Cocchi[1,2], Sonal Mistry[3], Martin Schmeisser[3], •Raymond Amador[1,2], Julius Kuehn[3], and Thorsten Kamps[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin, DE — [2]Humboldt-Universität zu Berlin, IRIS Adlershof, 12489 Berlin, DE — [3]Helmholz-Zentrum Berlin, 12489 Berlin, DE

The development of novel photocathode materials for ultra-bright electron sources demands understanding of intrinsic material properties, given constraints of growth and operational conditions. In a joint *ab initio* and experimental work, we propose a method to relate computed and measured core-level shifts and quantum efficiency of three alkali antimonides, which are particularly appealing for their absorption in the visible region. In our density-functional theory calculations we focus on Cs_3Sb, Cs_2KSb, and CsK_2Sb. Experimentally, Cs-K-Sb samples with different stoichiometries and relative elemental content are investigated using x-ray photoemission spectroscopy (XPS). The largest core-level shifts (2 eV and 0.5 eV for K 2*p* and Sb 3*d*, respectively) can be correlated to XPS survey spectra, where such peaks are clearly visible. Core-level shifts can thus be used to identify specific compositions of Cs-K-Sb materials and their relation to measured values of quantum efficiency. Our results represent the first step towards a robust connection between the experimental preparation and characterisation of photocathodes, the *ab initio* prediction of their electronic structure, and the modeling of emission and beam formation processes.

MM 42.5 Wed 16:45 IFW D

The effect of crystallinity of layered transition metal disulfide on the performance of potassium-ion batteries: The case of molybdenum disulfide — •Yulian Dong, Huaping Zhao, and Yong Lei — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Layer-structured transition metal dichalcogenides (LS-TMDs) are being studied in potassium-ion batteries owing to their structural uniqueness and electrochemical mechanisms. In this work, the dependence of electrochemical performance on the crystallinity of LS-TMDs has been investigated. Taking MoS2 as an example, lower crystallinity can alleviate diffusional limitation in 0.5*3.0 V, where intercalation reaction takes charge in storing K-ions. Higher crystallinity can ensure the structural stability of the MoS2 layers and promote surface charge storage in 0.01*3.0 V, where conversion reaction mainly contributes. The low-crystallized MoS2 exhibits an intercalation capacity (118 mAh/g) and great rate capability (41 mAh/g at 2 A/g), and the high-crystallized MoS2 delivers a high capacity of 330 mAh/g at 1 A/g and retains 161 mAh/g at 20 A/g. It shows that when intercalation and conversion reactions both contribute to store K-ions, higher crystallinity ensures the structural stability of the exfoliated MoS2 basal layers and promotes surface-controlled charge storage.

MM 43: Computational Materials Modelling - Alloys II

Time: Wednesday 17:15–18:30 Location: BAR 205

MM 43.1 Wed 17:15 BAR 205

Role of disorder in the electronic structure of thermoelectric clathrates — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

Intermetallic clathrate compounds have a huge compositional and configurational space that allows for tailoring their properties towards a high thermoelectric efficiency. For instance in $Ba_8Al_xSi_{46-x}$, the configuration of the Al atoms in the crystal framework drastically affects the electronic behavior [1]. This is most strikingly the case at the technologically relevant composition $x = 16$, whose ordered ground state is semiconducting, while disordered structures at higher energies are metallic. An in-depth understanding of this sensitivity of the electronic structure is crucial, since semiconducting behavior is a prerequisite for thermoelectric applications. In this work, we investiage the effects of disorder on the temperature-dependent electronic and structural properties. To this end, we develop a multi-scale approach, based on statistical thermodynamics combined with the cluster-expansion method [2] and *ab-initio* calculations. We discover a semiconductor-to-metal transition that is accompanied by an order-disorder phase transition at 582 K.

[1] M. Troppenz, S. Rigamonti, and C. Draxl, *Chem. Mater.* **29**, 2414 (2017).

[2] S. Rigamonti, *et al.*, `CELL`: python package for cluster expansions with a focus on complex alloys. URL: https://sol.physik.hu-berlin.de/cell

MM 43.2 Wed 17:30 BAR 205

High-temperature thermodynamics of Ni alloys with machine learning — •Nataliya Lopanitsyna and Michele Ceriotti — École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Many thermodynamic properties of metals show a pronounced temperature dependence that is challenging to obtain fully from ab initio. However, to achieve agreement between theoretical considerations and experiment, temperature-dependent contributions also should be taken into account. One of the problems is the absence of an accurate and efficient technique to obtain the correction. It becomes even more evident for properties such as the excess free energy associated with a solid-liquid interface which requires a number of atoms and simulation times unaccessible with electronic structure calculations. Interatomic potentials could be used to overcome computational expenses encountered in relation to ab initio methods. In this paper, to achieve high accuracy in the description of the interatomic interaction, we trained a neural network to approximate the potential energy surface defined by a solution of the Kohn Sham equation of DFT and incorporated it into free energy sampling techniques to quantify anharmonic effects appearing at high temperatures. We present a wide range of properties computed at finite temperature including elastic properties, bulk modulus, melting temperature, formation energies of single point defects, surface tension for nickel chosen as a representative of metal used for high-temperature applications. Additionally, we show the importance of having an accurate underlying interatomic potential by comparing fitted NNp to potentials reported in the literature.

MM 43.3 Wed 17:45 BAR 205

Machine trained interatomic potentials for multicomponent alloys — •Konstantin Gubaev[1], Yuji Ikeda[2], Fritz Körmann[1,2], Evgeny Podryabinkin[3], and Alexander Shapeev[3] — [1]Materials Science and Engineering, Delft University of Technology, 2628 CD, Delft, The Netherlands — [2]Computational Materials Design, Max-Planck-Institut fu*r Eisenforschung GmbH, 40237 Düsseldorf, Germany — [3]Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Nobel St. 3, Moscow, 143026, Russia

Accurate density-functional theory (DFT) calculations have become an indispensable tool in computational exploration and design of multicomponent alloys alas high entropy alloys (HEAs). The vastly unknown compositional and structural phase space of HEAs as well as the methodological obstacles related to the description of finite-temperature properties challenges the computational limits of standard DFT approaches and reveals the need for more efficient techniques.

Here we present DFT trained machine-learning potentials (MLIPs) as efficient force-fields for investigating finite-temperature properties of multicomponent alloys. The MLIP construction for a given alloy is performed within an iterative framework comprising the phase space sampling and subsequent MLIP training in an automated manner. As a result, MLIPs reconstructing the DFT atomic forces and total energies with unprecedented speed/accuracy combination are obtained. We demonstrate the approach by performing finite-temperature molecular-dynamics simulations to assess elastic properties of a set of bcc $\mathrm{TiZrHfTa}_x$ HEAs.

MM 43.4 Wed 18:00 BAR 205

Multi-scale Cluster Dynamics Modelling of Guinier–Preston Zone Formation in binary Al–Cu Alloys — •Tobias Stegmüller and Ferdinand Haider — Universität Augsburg, Institut für Physik, Universitätsstr. 1, 86159 Augsburg

The understanding of precipitation kinetics in modern age hardening aluminium alloys is, due to its significance on materials properties, of great technical interest. The link between ageing temperature and the evolution of the size distribution of precipitates is the key influence on material parameters like strength, hardness or corrosion resistance. Therefore the modelling of precipitation processes comes into focus to enable a quantitative prediction of the impact of ageing processes. For this purpose we developed a multi-scale model for the precipitation in binary alloys and tested it on the formation of Guinier–Preston zones (GPZ) in Al–Cu.

The approach results in the construction of a meso-scale Cluster Dynamics (CD) model, which is able to predict the evolution of the size distributions of the GPZ for different ageing temperatures and alloy compositions. Atomistic lattice Monte Carlo (MC) simulations were used to derive the necessary kinetic and thermodynamic input for CD. Finally, the smallest scale level includes density functional theory to derive a Cluster Expansion for the binary Al–Cu system, which provides the interaction parameters for our MC simulations. In addition, to validate the CD model, kinetic MC simulations on the formation of GPZ were conducted. The construction of the model as well as simulation results will be presented.

MM 43.5 Wed 18:15 BAR 205

Implementation of the coordination corrected enthalpies method into AFLOW — •Rico Friedrich[1], Marco Esters[1], Corey Oses[1], Demet Usanmaz[1], Cormac Toher[1], and Stefano Curtarolo[1,2] — [1]Center for Autonomous Materials Design, Duke University, USA — [2]Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, USA

The AFLOW database and software leverages *ab initio* calculations for autonomous materials design [1]. The predictive power critically relies on accurate formation enthalpies – quantifying the thermodynamic stability of a compound. For polar materials such as chalcogenides (*e.g.* oxides), pnictides (*e.g.* nitrides), and halides, standard semi-local DFT leads to errors of several hundred meV/atom [2,3].

We have recently developed the "coordination corrected enthalpies" (CCE) method yielding highly accurate room temperature formation enthalpies with mean absolute errors down to 27 meV/atom [3]. The approach is also capable of correcting the relative stability of polymorphs – an advantage versus earlier schemes. Here, we introduce a tool where users can input a structure file of their system and receive the CCE corrections, or even the CCE formation enthalpies if precalculated LDA, PBE or SCAN formation energies are provided. The results can be used for the computational design of polar compounds such as battery materials, defect systems, and high-entropy phases.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).
[3] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).

MM 44: Topical Session: Interface-dominated phenomena - Solutes at Interfaces II

Time: Wednesday 17:15–18:30 Location: IFW A

MM 44.1 Wed 17:15 IFW A

Atomic scale analysis on the elemental partitioning across phase boundaries in medium-Mn steels — •Wenwen Song, Yan Ma, and Wolfgang Bleck — Steel Institute (IEHK), RWTH Aachen University

The ultrafine grained medium-Mn steels (3˜12 wt.% Mn) emerge as a strong candidate for the 3rd generation of advanced high strength steels, due to its excellent mechanical properties. In the present work, we aim to understand the role of elemental partitioning across the interfaces, in particular the ferrite-austenite phase boundaries, during intercritical annealing and its impact on yielding behaviors. The nanostructured medium-Mn steels were characterized by atom probe tomography (APT), transmission electron microscopy (TEM) and high energy synchrotron x-ray diffraction (SYXRD). The 3D atomic maps show the elements concentration distribution. The elemental partitioning, i.e. C, Mn, Si, as well as the microalloy elements Nb, Mo, across the ferrite-austenite phase boundaries were analyzed. High carbon segregation at the ferrite-austenite phase boundaries were observed after intercritical annealing and air cooling. This segregation resulted in an increase in the yield strength and a pronounced discontinuous yielding phenomenon. The ferrite-austenite interfaces act as preferable nucleation sites for new partial dislocations in austenite and for full dislocations in ferrite. The current study sheds light on novel microstructural design and interface segregation strategies for ultrafine grained multiphase materials through phase-boundary engineering induced strengthening.

MM 44.2 Wed 17:30 IFW A

A quantum-mechanical study of clean and Cr-segregated antiphase boundaries in Fe_3Al — •Martin Friák, Monika Všianská, and Mojmír Šob — Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

We present a quantum-mechanical study of thermodynamic, structural, elastic, and magnetic properties of selected antiphase boundaries (APBs) in Fe_3Al with the $D0_3$ crystal structure with and without Cr atoms. The computed APBs are sharp (not thermal), and they have {001} crystallographic orientation. They are characterized by a mutual shift of grains by $1/2\langle 100\rangle$, i.e., they affect the next nearest neighbors (APB-NNN type, also called APB-$D0_3$). Regarding clean APBs in Fe_3Al, the studied ones have only a very minor impact on the structural and magnetic properties, including local magnetic moments, and the APB energy is rather low, about 80 mJ/m^2. Interestingly, the studied APBs play a crucial role in the anisotropic (tensorial) elastic properties. The Cr atoms have a strong impact on magnetic properties and a complex influence on the energetics of APBs. The Cr atoms in Fe_3Al exhibit clustering tendencies even in the presence of APBs and cause a transition from a ferromagnetic into a ferrimagnetic state. The impact of Cr atoms on APB energies in Fe_3Al is found to be ambiguous, including reduction, having a negligible influence or increasing APB energies depending on the local atomic configuration of Cr atoms. As similarly contradicting trends were found in experiments, our results can shed a new light on these experimental data (see M. Friák, M. Všianská, M. Šob, Materials 12 (2019) 3954).

MM 44.3 Wed 17:45 IFW A

Ag segregation induced nanofaceting transition of a Cu tilt grain boundary and its impact on plastic deformation mechanisms — •Nicolas J. Peter, Christian H. Liebscher, Christoph Kirchlechner, and Gerhard Dehm — Max-Planck Insitut für Eisenforschung GmbH

We describe the observation of a nanofaceting transition of an asymmetric tilt GB in Cu upon Ag segregation by atomically resolved scanning transmission electron microscopy. The initially flat {110}/{410} boundary was found to dissociate into Ag-lean {230}/{100} asymmetric facet segments and Ag-rich symmetric {210} segments. Thus, a preferential segregation pattern of stable nanosized facets was found. Further, the influence of Ag solute excess concentration on the facet formation was studied by a diffusion couple. It was found that the asymmetric segment remains constant in size, while the symmetric facet segment increases with increasing solute excess. At the diffusion couple's interface a purely symmetric {210} boundary is found. Following the GB, short asymmetric facet segments are introduced and increase their density until a purely asymmetric GB is found close to the non-segregated reference state. Finally, we linked the observed faceting transition to a change in plastic deformation behaviour by tensile straining GB containing bicrystals in situ inside the electron microscope. While pure Cu reference boundaries deform by local emission of partial dislocations resulting in the formation of a single deformation twin, the Ag segregated bicrystal shows numerous partial dislocation nucleation sites resulting in an increase of deformation twins.

MM 44.4 Wed 18:00 IFW A

Influence of impurities on the grain boundary strength in Ir — •Minaam Qamar, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

The present work aims to explore the role of segregated impurities on the grain boundary strength in iridium. Ab initio tensile tests were performed on both pure and impurity-segregated high angle symmetric tilt grain boundaries (GBs) and their cohesive strengths were compared. Two distinct GBs, $\Sigma5(210)[001]$ and $\Sigma11(113)[110]$, were chosen for the study with segregated H and Si atoms. The GBs show a contrasting behavior with respect to trapping sites of the impurity atoms: while the relatively loosely packed $\Sigma5$ GB has multiple low energy trapping sites, the close-packed $\Sigma11$ GB has very few. The behavior of the impurities is also markedly different: Si atoms show a much stronger segregation than H atoms. In addition, a detailed analysis of the migration of an H atom through the GBs found that the arrangement of atoms provides an easy migration path into the GB plane and a high energy barrier for reverse migration, effectively trapping the atom in the GB. However, despite the favorable segregation, neither H nor Si do not seem to significantly affect the cohesive properties of the GBs.

MM 44.5 Wed 18:15 IFW A

Microscopic understanding of Zn diffusion in Fe grain boundaries. — •Michael Geier[2], Martin Panholzer[1], Martin Hoffmann[1], Heiko Groiss[2], Kurt Hingerl[1], and Robert E. Zillich[1] — [1]Johannes Kepler University, Linz, Austria — [2]Christian Doppler Laboratory for Nanoscale Phase Transformations, Center for Surface and Nanoanalytics, Johannes Kepler University, Linz, Austria

Zn coatings are widely used for corrosion protection of steel. However, Zn can lead to a weakening of steel grain boundaries during steel processing at higher temperatures. To investigate this liquid metal embrittlement in the presence of liquid zinc, the diffusing properties of a single Zn atom in Fe grain boundaries were studied using density functional theory which treat the Zn-Fe interactions very accurately. In our approach, we built a simple bcc Fe grain boundary or a dislocation in bcc Fe, and placed a Zn atom within both. With the nudged elastic band method we calculated the energy barrier which the Zn atom has to overcome for moving along the grain boundary or dislocation. Additionally we calculated with transition state theory and random walk theory the diffusion coefficient of the one dimensional diffusion of Zn along the grain boundary. Our results show that the Zn atom diffusion depends strongly on the type of lattice defect, i.e. grain boundary or dislocation. However, it turns out that the difference decreases when approaching melting temperature.

MM 45: Computational Materials Modelling - Low dimensional systems

Time: Wednesday 17:15–18:30 Location: IFW B

MM 45.1 Wed 17:15 IFW B

Density functional theory of structural distortion in one dimensional and three dimensional structures — Uri Argaman, Daniela Kartoon, and •Guy Makov — Dept. of Materials, Ben-Gurion University, Beer-Sheva, Israel

The onset of distortion in one-dimensional monatomic chains with partially filled valence bands is considered to be well established by the Peierls theorem, which associates the distortion with the formation of a band gap and a subsequent gain in energy. Many half-filled p-band materials form complex, semiconducting or semi-metallic crystallographic structures, which are commonly conceived of as distortions of simpler, higher-symmetry structures. Employing modern total energy methods on the test cases of elemental chains and lattices, we reveal that the distortion is not universal but conditional upon the balance between distorting and stabilizing forces. Furthermore, in all systems studied, the electrostatic interactions between the electrons and ions act as the main driving force for distortion, rather than the electron band lowering at the Fermi level as is commonly believed. The main stabilizing force which drives the structures towards their symmetric arrangement is the electronic kinetic energy. Both forces are affected by the external conditions, e.g., stress, and consequently the instability is conditional upon them. These results may shed light on the distortion of more complex structures. Funding Acknowledgement: Support of the Israel Ministry of Science and Technology is acknowledged.

MM 45.2 Wed 17:30 IFW B

Ab initio study of partial basal dislocations in bilayer

graphene and few-layer graphene — •Pavlos Mouratidis[1], James McHugh[1], Kenny Jolley[1], Malcolm Heggie[1], and Patrick Briddon[2] — [1]Department of Chemistry, Loughborough University, Loughborough, United Kingdom — [2]Newcastle University, School of Engineering, Newcatsle upon Tyne, United Kingdom

Graphite has been the material of choice in construction of nuclear reactors for many years due to its low neutron absorption cross-section and high scattering cross-section. The physical properties of a graphite moderator can greatly influence the cost, safety and lifespan of a reactor. Neutron collision damage in graphite results in the formation of basal dislocations. The subsequent interaction of basal dislocations with each other and the surrounding lattice causes severe dimensional changes along the basal direction.

There has been a lot of interest recently in AB and AC stacking grain boundaries in bilayer graphene. Transition from AB to AC stacking can be described by the glide of partial basal dislocations resulting in expansion of dislocation cores and buckling of the bilayer. Herein we present full ab initio and molecular dynamics calculations of basal dislocation network structures in bilayer graphene and few-layer graphene in large supercells of up to 100 nm.

MM 45.3 Wed 17:45 IFW B

Continuum modeling of complex solid-state dewetting scenarios by the phase-field method — •Marco Salvalaglio and Axel Voigt — Institute of Scientific Computing, TU Dresden

Solid-state dewetting is a process through which continuous solid films break and agglomerate to form separated islands. It is a spontaneous phenomenon driven by surface energy minimization, which can occur in thin films via surface diffusion at high temperatures. Although being detrimental during the processing of planar architectures, it may be exploited to obtain a large variety of self-assembled structures in a controlled fashion, such as droplets, nanowires, connected filaments, and pierced films. We present the continuum, phase-field modeling of surface diffusion applied to the study of solid-state dewetting. In particular, the case of monocrystalline films undergoing dewetting on amorphous substrates is addressed, including relevant physical contributions such as surface-energy anisotropy and elasticity effects. The standard approach is discussed, along with recent model improvements. Numerical simulations are shown to reproduce and predict the outcome of annealing experiments for patterned silicon-on-insulator films leading to complex nano-architectures and ultra-long nanowires. Moreover, they assess the role of elasticity in enabling a spinodal solid-state dewetting regime during the annealing of strained thin-crystalline films lying on amorphous substrates.

MM 45.4 Wed 18:00 IFW B

sp3 Bonded 2-Dimensional Allotrope of Carbon: A First-Principles Prediction — •Bikram Kumar Das, Dipayan Sen, and Kalyan Kumar Chattopadhyay — Thin Film and Nanoscience Laboratory, Department of Physics, Jadavpur University, Kolkata, India

In this work, using state-of-the-art theoretical calculations, we considered cyclobutane motifs, and investigated whether a sp3 bonded 2-dimensional carbon allotrope could be achieved by assembling ladderane chains. Energetic and dynamic stability studies yielded two such promising structures: one with 4-coordinated carbon atoms, space group PMMA, and a relatively more stable structure with a combination of 3 and 4-coordinated carbon atoms, space group P2/C; both having puckered geometries and partially sp3 C-C bonds. However thermal stability investigations indicated only the lower energy configuration could be stable at ambient temperature and pressure. Electronic structures of the proposed allotropes were studied with density functional theory at rigorous HSE06 level. Investigation of electronic properties of these proposed materials revealed them to be direct-gap semiconductors with small bandgaps. Under in-plane biaxial compressive strains, bandgaps of both were found to decrease; whereas, under similar tensile strains, bandgaps of both were observed to increase up to a strain limit of 5% and 6% for Phase 1 and 2 respectively.The predicted small bandgap values of the proposed allotropes, and especially their convenient tunability is thus highly promising from the perspective of next-generation carbon based microelectronics applications.

MM 45.5 Wed 18:15 IFW B

Prediction of two-dimensional square-A_2B (A=Cu, Ag, Au, and B=S, Se) auxetic semiconductors with ultra-high negative Poisson*s ratios and unusually low lattice thermal conductivities — •Xin Chen[1], Duo Wang[1], Xiaobiao Liu[2], Linyang Li[3], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, 751,20 Uppsala, Sweden — [2]School of Sciences, Henan Agricultural University, Zhengzhou 450002, PR China — [3]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

Using evolutionary crystal structure search and density functional calculations, we have obtained two-dimensional (2D) structures of A_2B (A=Cu, Ag, Au, and B=S, Se). Structural, electronic and mechanical properties of the global minimum single-layer A_2B structures were studied in detail. These structures have two types of geometries (s(I) and s(II)) with square symmetry, and are named square-A_2B (s-A_2B or s(I/II)-A_2B) in this paper. All of the s-A_2B structures are semiconductors with direct bandgaps ranging from 1.09 eV to 2.60 eV. Due to the ionic bonding nature, 2D s-A_2B structures have unusually low lattice thermal conductivities, down to 1.5 Wm*1K*1 at room temperature. Also, s-A_2B structures have ultra-low Young*s moduli, which are lower than most previously reported 2D materials, showing their extraordinary flexibility. Moreover, under the application of strain along the diagonal direction, five of these structuers show in-plane negative Poisson*s ratio (NPR). In particular, the NPR of s(II)-Cu2S can reach up to -1.68, higher than other predicted auxetic materials.

MM 46: Materials for Energy Storage and Conversion - Electronic Properties

Time: Wednesday 17:15–18:30 Location: IFW D

MM 46.1 Wed 17:15 IFW D

Oxygen Vacancy Formation and Diffusion in Oxide Electrode Materials for High-Temperature Electrolysis — •Hanna Tuerk, Karsten Reuter, and Christoph Scheurer — Technical University of Munich

In a sustainable energy system, the intermittency of green electricity needs to be addressed. One possible solution to stabilize the grid are solid-oxide electrolyzer cells (SOECs), which are able to store excess electric energy into hydrogen on demand [1]. While such high-temperature SOECs are in principle well adapted to intermittent operation with frequent start-ups and shut-downs, cell performance and lifetime of existing SOECs is severely limited by anode degradation [2].

This degradation goes hand in hand with the oxygen evolution reaction (OER) taking place at the triple-phase boundary between the electrode, the electrolyte and the gas phase. In order to shed light on this degradation mechanism, oxygen vacancy formation and defect mobility at the interface of the standard electrolyte yttria-stabilized zirconia (YSZ) and the typical electrode material strontium doped lanthanum manganite (LSM) are investigated theoretically. The structural complexity of the active catalyst region mandates the use of an efficient polarizable force field, which is able to provide insight into the atomistic processes at the higly disordered interface.

[1] S. Foit *et al.*, Angew. Chem. Int. Ed. 56, 5402 (2017).

[2] M. S. Sohal *et al.*, J. Fuel Cell Sci. Tech. 9, 011017 (2012).

MM 46.2 Wed 17:30 IFW D

An ultrafast graphite oxide-graphite capacitor enabled by potassium-based ether electrolyte — •Chenglin Zhang, Long Liu, Yuhan Wu, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Graphite oxide-graphite hybrid capacitor which can offer energy between batteries and supercapacitors while in principle offering supercapacitor-like power and cyclability values was proposed as a supplementary to batteries. This prototype not only explores cheaper potassium to replace lithium to reduce costs but also employ mature commercial graphite as the negative electrode and its derivative as the positive electrode to further reduce costs and improve the prospect of commercialization. The potassium-based ether electrolyte was demonstrated that can perfectly comply with both fast ion adsorption on the graphite oxide cathode and co-intercalation in graphite anode. The extremely low-cost carbonaceous capacitor exhibited outstanding performance with large capacity, high rate capability, and long cyclability. Considering the cost-effectiveness, material sustainability, this new model may shed some light on searching for future energy storage devices.

MM 46.3 Wed 17:45 IFW D

Investigating the Role of Nanoarchitectured Current Collector in Supercapacitor Electrode with Thick Pseudocapacitive Materials — •Long Liu, Huaping Zhao, Mo Sha, Chenglin Zhang, Jiajia Qiu, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Pseudocapacitive materials with low electrical conductivity are mainly in the form of ultrathin conformal coating in supercapacitor electrodes based on nanoarchitectured current collectors, thus the resultant low mass loading of electroactive materials largely limits the applications of nanoarchitectured current collectors. Here, supercapacitor electrodes with nickel nanorod arrays as nanoarchitectured current collectors and MnO2 as electroactive materials are fabricated to investigate the role of nanoarchitectured current collectors in determining the energy storage capability when pseudocapacitive materials are in thick layer rather than ultrathin conformal coating. Electrochemical analysis revealed that Ni nanorods could create numerous electrical conductive tunnels in the thick-layer electrodes to dramatically alleviate the contact resistance at the electroactive-materials/current-collectors interface. Larger area capacitance, better rate capability and higher structural stability was maintained in Ni nanorods based electrodes even with thick MnO2 layer than those with Ni foils as current collectors based electrode with the same configuration. These results open up new opportunities for nanoarchitectured current collectors to construct supercapacitors with superior energy storage capability.

MM 46.4 Wed 18:00 IFW D

Phase Stability Diagrams of Group 6 Magnéli Oxides and Their Implications for Photon-Assisted Applications — •Yun-Jae Lee, Taehun Lee, and Aloysius Soon — Department of Materials Science & Engineering and Center for Artificial Synesthesia Materials Discovery, Yonsei University, Seoul 03722, Republic of Korea

Controlling the stoichiometry and metastability in functional oxides is often the key to enhancing their performance for a range of important oxide-based technological applications. In this work, using the recently developed metaGGA, SCAN+rVV10, and hybrid density-functional theory calculations, we study both stoichiometric and sub-stoichiometric (Magnéli) oxides of tungsten and molybdenum, focusing on their structural parameters, growth thermodynamics, and electronic structure for targeted photo-related applications. We report that the sub-stoichiometric Magnéli phases of tungsten oxides (namely, W_5O_{14} and $W_{18}O_{49}$) are found to be stable under both gas- and solution-based synthesis environment, while the sub-stoichiometric Magnéli phases of molybdenum oxides (namely, Mo_9O_{26}, Mo_5O_{14}, and Mo_4O_{11}) prefer to form only under gas-phase synthesis. We highlight how these n-doped sub-stoichiometric Magnéli heavy-metal oxides are indeed choice candidate materials for solar water splitting (within the Z-scheme) and as interfacial hole transport layers for the next-generation photodevices.

MM 46.5 Wed 18:15 IFW D

Lattice dynamics in PbTe under high pressure — •Zehua Li[1], Shasha Li[2], Rolf Heid[1], John-paul Castellan[3], Stefan Klotz[4], Alexandre Ivanov[5], Yue Chen[2], and Frank Weber[1] — [1]Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe, Germany — [2]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China. — [3]Laboratoire Léon Brillouin (CEA-CNRS), CEA-Saclay, F-91911 Gif-sur-Yvette, France — [4]Sorbonne Université, UMR 7590, IMPMC, F-75252 Paris, France — [5]Institut Laue-Langevin, 71 avenue des Martyrs, 38000 Grenoble, France

Thermoelectric materials such as PbTe are interesting for energy applications as they can transform heat into useful electricity. Understanding the impact of anharmonicity in the lattice dynamical properties is the key to engineer/design new high-performance thermoelectric materials requiring a low lattice contribution to the thermal conductivity. Here, we report an investigation on zone center transverse optic phonons in PbTe at pressures up to 5.3 GPa by inelastic neutron scattering. We observe a non-monotonic pressure dependence in the phonon energy as well as a clearly reduced phonon linewidth at high pressures.

MM 47: Annual General Meeting

Time: Wednesday 18:30–20:00 Location: IFW A

Duration: 90 min.

MM 48: Invited talk Gunkelmann

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

Invited Talk MM 48.1 Thu 9:30 BAR 205

Molecular dynamics simulations of pressure induced phase transformations in iron and iron-carbon: Interplay of defects and phase transition — •Nina Gunkelmann[1], Hoang-Thien Luu[1], Ramon J. Ravelo[2], Timothy C. Germann[3], Eduardo M. Bringa[4], and Herbert M. Urbassek[5] — [1]TU Clausthal, Germany — [2]University of Texas, El Paso, USA — [3]Los Alamos National Laboratory, USA — [4]University of Mendoza, Argentina — [5]TU Kaiserslautern, Germany

The study of iron under high-pressure conditions is essential not only for industrial activities but also for geological and astronomical applications. We consider iron and iron-carbon alloys showing a pressure induced phase transformation from the bcc to the hexagonal close-packed phase at around 13 GPa depending on the carbon content. We study compression waves in polycrystalline Fe and Fe-C using interatomic potentials that faithfully incorporate this phase transition at the desired equilibrium pressure. Our simulations show that the phase transformation is preceded by plastic activity, leading to the so-called 3-wave structure: An elastic compression wave is followed by a plastic wave, which then leads to a phase-transformation front. We investigate the interplay of defects in bcc with the transformation process. The role of twins, dislocations, and Cottrell atmospheres has a strong influence on the crystalline iron structure during the phase transformation. Our results show that the presence of Cottrell atmospheres surrounding an edge dislocation in bcc iron retards the development of the hcp phase.

MM 49: Structural Materials (Steels, light-weight materials, high-temperature materials) - I

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

MM 49.1 Thu 10:15 BAR 205

First principles study on hydrogen behaviour in Cr and Mn containing carbides of high Mn steels — •Lekshmi Sreekala, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237, Düsseldorf

Understanding hydrogen-assisted embrittlement of advanced high-strength steels is decisive for their application in automotive industry. Since the addition of Cr to the composition of high-Mn steels improves their corrosion resistance and simultaneously changes the microstructure, the influence of Cr and Mn on hydrogen solubility in the context of carbide formation is scientifically challenging. Density functional theory based calculations have been employed to determine the thermodynamic driving force for the formation of carbides as a function of the chemical composition of the alloy and also to study hydrogen interaction of carbides and interfaces containing Cr and Mn. Our results show that Cr has an indirect impact on hydrogen, since it strongly influences the thermal stability of the carbides like cementite and $Fe_{23}C_6$. However, the individual Cr atom interacts only weakly with H. On the other hand, Mn has a weaker impact on carbide formation. However, its incorporation into the carbides yields a remarkably strong non-linear interaction with hydrogen, qualitatively different from the known H-Mn interaction in the austenitic steel matrix.

MM 49.2 Thu 10:30 BAR 205

Interaction of helium, self-interstitial atoms and vacancies with YTiO clusters in bcc Fe — •Muthu Vallinayagam[1,2], Matthias Posselt[1], and Jürgen Fassbender[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf,Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400,01328 Dresden,Germany — [2]Technische Universität Dresden,01062 Dresden,Germany

In nanostructured ferritic/martensitic Fe-Cr alloys YTiO clusters act as sinks for the irradiation-induced defects He, self-interstitial atoms(SIA), and vacancies(v). In this manner, irradiation swelling can be retarded significantly. In this ab-initio simulation work, interactions of He and other defects with YTiO cluster in bcc Fe are investigated considering cluster structures studied in a previous work[1]. It is found that the most stable position of He is in the center of the cluster, then interfacial vacant sites and other interstitial positions between metal or oxygen atoms, and sites away from the cluster[2]. Calculations on the addition of two and three He atoms to the cluster show that the total binding energy is equal to the sum of binding energies of individual He atoms. Therefore, He trapping depends mainly on the availability of regions with low electron density. A significant attraction between cluster and SIA is observed. This results in annihilation of SIA due to the existence of interfacial vacant sites. Vacancies are also trapped by YTiO clusters and their binding energy increases if the vacancy approaches O terminated sites. [1]Vallinayagam et al 2019 J. Phys.: Condens. Matter 31 095701 [2]Vallinayagam et al 2019 J. Phys.: Condens.Matter 31 485702

MM 49.3 Thu 10:45 BAR 205

Effect of Re and Os on the 1/2$< 111 >$ dislocations in W — •Aparna P. A. Subramanyam, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universität-Bochum, Bochum, Germany

W is the prime candidate for plasma facing first wall material in fusion reactors. The neutron bombardment causes nuclear transmutation of W atoms to Re and Os atoms which affect the mechanical properties of the material. In order to understand these effects, we perform large-scale atomistic simulations with a recently developed analytic bond-order potential (BOP) for the ternary W-Re-Os system. This tight-binding based BOP provides a robust description of the underlying electronic structure and is validated against available experimental and ab-initio data. Here, we discuss the effects of Re and Os on the energetics and local atomic structure of the $1/2 < 111 >$ edge and screw dislocations in W. We also analyze the motion of these dislocations in pure W as well as in W-Re and W-Os alloys in terms of Peierls stresses and discuss the influence of these elements on the kink pair formation energy in W.

MM 49.4 Thu 11:00 BAR 205

Effect of additive materials on chlorine induced high temperature corrosion in waste-to-energy plants — •Sebastian Pentz[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 to massive problems especially in waste-to-energy-plants. At prevalent temperatures around 400°C-600°C, corrosion is mainly chlorine induced. A local release of chlorine through sulfation reaction of solid alkali chlorides is mainly responsible for the supply of chlorine at metallic components like superheaters. This reaction requires an atmosphere containing SO_2, H_2O, O_2 and releases HCl/Cl_2. Sulfates thereby generated could in combination with deposited chlorides lead to low melting eutectics in the deposit concluding in an acceleration of the corrosion process. A strategy with good prospects could be the application of additive materials in order to confine the chloride deposition. In this work the absorbing mechanism of clay minerals is examined. The additive kaolinite enables the incorporation of alkalis like Na or K. Hereby chlorine is released as gaseous HCl leading to less condensation of NaCl/KCl. Hence chlorine enrichment in the deposits can be reduced. Principles of the reaction conditions in waste-to-energy-plants, especially at the superheater tubes, are investigated and laboratory experiments regarding the encapsulation of alkalies into clay minerals, the kinetics of sulfation reactions and the corresponding chlorine attack are evaluated.

MM 49.5 Thu 11:15 BAR 205

$CeMo_2B_5$: a new type of arrangement of puckered boron hexagonal rings — •Sever Flipo[1,2], Miroslav Kohout[2], Friedrich Roth[1], Tina Weigel[1], Matej Bobnar[2], Alim Ormeci[1,2], Ulrich Burkhardt[2], Christoph Hennig[3], Tilmann Leisegang[1], Dirk Carl Meyer[1], Andreas Leithe-Jasper[2], and Roman Gumeniuk[1,2] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany — [3]ESRF, 71, Avenue des Martyrs, Grenoble, France

$REMo_2B_5$ (RE = Ce, Pr, Nd) and CeW_2B_5 have been synthesized. $CeMo_2B_5$ crystallizes in a new structure type with space group *Pnma*, $a = 11.0298(2)$ Å, $b = 3.12080(5)$ Å, $c = 9.9594(2)$ Å, $Z = 4$. Its structure reveals puckered [B6]-hexagonal rings, trigonal-prismatic- and empty slabs of condensed pyramids and tetrahedra. The structure can be related to the derivatives of AlB_2 and CrB prototypes. The boron atoms form a two-dimensional network of corrugated ribbons, each composed of four edge-linked [B6] rings extending infinitely along the *b*-axis. The Chemical bonding scenario in $CeMo_2B_5$ is dominated by the chains of [Ce2Mo2] clusters with multi-center bond. These clusters are connected via metallic Mo*Mo bonds and the resulting framework is stabilized by bonding interactions with the boron ribbons to which it donates electrons. $CeMo_2B_5$ is a Pauli paramagnet and electrical transport measurements, as well as the calculated density of states at the Fermi level, show $CeMo_2B_5$ to be a typical metallic system.

MM 50: Topical Session: Interface-dominated phenomena - Thermodynamics and Microstructure Evolution

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

Topical Talk MM 50.1 Thu 10:15 IFW A

A Density-based Model for Grain Boundary Thermodynamics and Kinetics — •Reza Darvishi Kamachali, Lei Wang, and David Jacobson — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

Despite their nonequilibrium nature, grain boundaries can have lasting effects on the alloys microstructure, especially when interacting with solute atoms. In fact, solute segregation to grain boundaries is identified as a tool for microstructure design. To make the most of its potentials, a quantitative understanding of grain boundary segregation is required. We propose here a model for studying phase stability and microstructure evolution at grain boundaries. A continuous density field and its corresponding gradients are considered to derive grain boundary thermodynamic functions based on available bulk thermodynamic data. Grain boundary equilibrium phase diagrams are obtained. Several results on segregation and phase separation in binary and ternary alloy systems will be discussed. Based on the current model, some new aspects of grain boundary kinetics and solute drag will be presented as well. The current density-based model for grain boundaries can be readily applied for studying and design of polycrystalline materials.

References: [1] Kamachali RD. A Model for Grain Boundary Thermodynamics. ArXiv: arXiv:1907.12231. 2019. [2] Kamachali RD, da Silva AK, McEniry E, Ponge D, Gault B, Neugebauer J, Raabe D. Segregation–Assisted Spinodal and Transient Spinodal Phase Separation at Grain Boundaries. arXiv:1905.07970. 2019.

MM 50.2 Thu 10:45 IFW A

Effect of thermally driven phase separation on the (nanoscale) magnetic properties of Fe-Cr — •Vladimir Vojtech[1], Robin Schäublin[1], Severin Küchler[1], Andras Kovacs[2], Rafal Dunin-Borkowski[2], and Jörg Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Peter Grünberg Institute, Forschungszentrum Jülich, Germany

Ferritic steel is one of the most promising candidates for deployment as structural material in future fusion reactors. However, the harsh operation conditions, with high temperatures and neutron irradiation, will degrade these materials. In particular, ferritic steel can undergo phase separation leading to Cr-rich α' precipitation, which hardens and embrittles the alloy and may change its magnetic nature. As technological ferritic steels are complex in microstructure and chemistry, studies on fundamental microstructural mechanisms are usually conducted on Fe*Cr model alloys. In this work, we study the thermally driven decomposition in the Fe*Cr system with Cr amounts ranging from 5 to 40 wt.% and annealed for 50 hours to 3 months at 500 °C. Scanning transmission electron microscopy (TEM) with energy-dispersive X-ray spectrometry was used to chemically map the α' phase, while magnetometry, Lorentz TEM and electron holography were deployed to study its impact on the magnetic properties. We will discuss in detail the observed pronounced effect of the decomposition on the magnetic domain size.

MM 50.3 Thu 11:00 IFW A

Thermodynamics, atomic and electronic structure of pristine and doped wurtzite ZnO(0001) inversion domain boundaries — •Jochen Rohrer and Karsten Albe — Institut für Materialwissenschaft, Fachbereich Materialwissenschaft, Technische Universität Darmstadt, Germany

ZnO bicrystal samples with (0001)||(0001) and $(000\bar{1})|(000\bar{1})$ inversion domain boundaries (IDB) show strong variations in conductivity with respect to strain which is attributed to a modulation of the barrier height of the electric potential [1]. In this contribution, we aim at gaining atomistic insight into this phenomena using electronic-structure calculations coupled to thermodynamic analysis.

In particular, we present a comprehensive study on prisinte and doped IDBs considering a large variety of structurally and chemically different model geometries. Despite the lack of inversion symmetry we compute individual grain boundary excess energies by an appropriate choice of model geometries. These models contain one IDB and additional surfaces whose excess is calculated separately and then subtracted. For thermodynamically favoured systems we then investigate electronic structure and repsonse to applied strain in detail.

[1] P. Keil *et al.*, *Adv. Mater.* **30**, 1705573 (2018).

MM 50.4 Thu 11:15 IFW A

Atomistic modeling of the influence of precipitates on the yield strength in Al-Ni-Zr eutectic alloys — •Daniel Mutter[1], Johannes Preussner[1], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Lightweight construction is important to achieve resource efficient design, particularily in the mobility sector to reduce fuel combustion and CO$_2$ emission. In order to fulfill the weight, stability and safety requirements, the materials for this purpose have to be light and at the same time exhibit high specific yield strengths. Al is the most important element in this context, and the existence of a eutectic point in many binary Al-alloys (such as Al-Si, Al-Ni or Al-Ca) further facilitates production processes and leads to alloys with good mechanical properties. By including small amounts of additional elements to the eutectic composition and cooling the melt below the critical temperature, finely dispersed intermetallic phases can form. Their existence within the Al matrix has a strong influence on the mobility of dislocations and can strengthen the material considerably (precipitation hardening). Here, we present results of atomistic modeling and simulation of underlying effects in the Al-Ni system with Zr additives, such as anti-phase boundary energies or shear moduli mismatches between the matrix (fcc-Al) and the precipitate phase, which was shown to consist of L1$_2$ ordered Al$_3$Zr. The properties and a possible influence of the phase boundary between matrix and eutectic phase (Al$_3$Ni) are also discussed.

MM 51: Computational Materials Modelling - Mechanical Properties

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

MM 51.1 Thu 10:15 IFW B

Atomic scale investigation of internal friction in austenitic steels — •Osamu Waseda, Tilmann Hickel, and Jörg Neugebauer — MPIE Düsseldorf

Internal friction measurements are a powerful method for the identification of the nature of point defects and complex short range order of solute atoms in austenitic steels. Whereas it is possible to identify point defect interactions that contribute to internal friction, it is difficult to decompose experimental results into each cause, as the complex interactions and the stochastic nature of solute diffusion smear out different contributions. Therefore, the interpretation of experimental results requires assumptions that are currently a matter of discussion. Correspondingly, a theoretical model that yields quantitative agreement with experiments is still missing for austenite. In this study, we developed a novel thermodynamic method conjugated with ab initio calculations to understand the short range ordering generated by vacancies and carbon atoms. This model not only accounts for the variation of solute interactions due to material deformation, but also the variation of migration energies due to solute interactions. In this way, it removes the commonly known discrepancy between empirical models and experimental results. This model, therefore, enables us to decompose experimental internal friction results into each contribution of point defect interactions. This clarifies the nature of short range order of carbon and vacancies in austenite, which is decisive for their mechanical performance.

MM 51.2 Thu 10:30 IFW B

Closing the gap between atomic-scale lattice deformations and continuum elasticity within the phase-field crystal framework — •Marco Salvalaglio[1], Ken Elder[2], and Axel Voigt[1] — [1]Institute of Scientific Computing, TU Dresden — [2]Department of Physics, Oakland University, Rochester, Michigan, USA

The Phase-Field Crystal (PFC) model allows for describing atoms in a lattice through a continuous probability density and focusing on diffusive time scales. In the amplitude expansion of the PFC model (APFC), a coarse-grained description of the atomic probability density is obtained by focusing on its complex amplitudes and, in turn, on their dynamics. These amplitudes vary on length scales larger than the atomic spacing but still retain details of the crystal lattice. Numerical simulations based on the APFC model and exploiting the Finite Element Method are shown to reproduce defects structures in two and three dimensions for different crystal symmetries as well as their dynamics. The derivation of continuous deformation fields from the complex amplitudes, their connections with the elasticity theory, and the characterization of dislocations by the Burgers vector density are also discussed. These findings assess the APFC model as a reliable coarse-graining of the PFC model. More importantly, the description of crystal structures through amplitudes is shown to provide a natural framework connecting atomic-scale lattice deformations and continuum elasticity.

MM 51.3 Thu 10:45 IFW B

Two mechanisms of anomalous slip in bcc metals — •Roman Gröger[1] and Vaclav Vitek[2] — [1]Czech Academy of Sciences, Institute of Physics of Materials and CEITEC IPM, Brno, Czech Republic — [2]University of Pennsylvania, Department of Materials Science and Engineering, Philadelphia, PA, USA

Many body-centered cubic metals and alloys exhibit anomalous slip of $1/2\langle 111\rangle$ screw dislocations on $\{110\}$ planes with very low Schmid factors. The origin of this phenomenon is still unknown but there is a growing pool of evidence linking it to core structures of these dislocations and their transformations under applied load. Here, we identify two possible mechanisms leading to the anomalous slip for uniaxial loading in the center of the stereographic triangle. The first originates from the glide of $1/2[111]$ and $1/2[\bar{1}11]$ screw dislocations on their most highly stressed planes, as proposed by the Schmid law. This inevitably leads to their intersection and formation of $[100]$ screw junctions, as proposed previously in the co-planar double slip model. If this junction is strong, the three dislocations have to move on their common $(0\bar{1}1)$ plane, which results in anomalous slip. The second mechanism is based on a hypothesis that the two $1/2\langle 111\rangle$ screw dislocations may move directly on the $(0\bar{1}1)$ plane in contradiction to the Schmid law. Using atomistic simulations, we investigate which of these two mechanisms is operative at 0 K in the five non-magnetic bcc metals (V, Nb, Ta, Mo, W), magnetically isotropic state of Cr, and in ferromagnetic α-Fe. The predictions of both models are compared with available low-temperature experiments on high-purity single crystals.

MM 51.4 Thu 11:00 IFW B

Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys — •Shihao Zhang[1,2], Yuanqi Guo[1], Irene J. Beyerlein[3], Dominik Legut[2], Shunli Shang[4], Zi-Kui Liu[4], and Ruifeng Zhang[1] — [1]School of Mat. Sci. and Eng., Beihang University, China — [2]IT4Innovations, VSB-TU Ostrava, Czech Republic — [3]University of California at Santa Barbara, USA — [4]Pennsylvania State University, USA

Zn and Mg alloys are considered highly promising biodegradable materials for cardiovascular stent applications; however, their poor strength has prevented this application. Via first-principles calculations and Peierls-Nabarro model, we investigate the coupled effect of the solute element and mechanical straining on the stacking fault energy (SFE), dislocation core structure, and Peierls stress in Zn and Mg alloys. Several biocompatible solute, i.e., Li, Al, Mn, Fe, Cu, Mg and Zn, were considered. It is suggested that some elements, like Fe, can potentially enhance strength in both Zn and Mg alloys, while other elements, like Li, can lead to opposed effects. The effect of solute strengthening and longitudinal straining on SFEs is much stronger for the Zn alloys than for the Mg alloys. Investigations on electronic structure and bond lengths reveal a coupled chemical-mechanical effect of solute and strain on electronic polarization, charge transfer, and bonding strength, which can explain the weak mechanical effect on Zn alloys and the variable strengthening effect among these solutes. These findings provide critical information needed in solute selection in Zn and Mg alloy design for biomedical applications.

MM 51.5 Thu 11:15 IFW B

The emergence of small-scale self-affine surface roughness from deformation — •Wolfram Nöhring[1], Adam Hinkle[1,2], Richard Leute[1], Till Junge[6], and Lars Pastewka[1,3,4,5] — [1]Department of Microsystems Engineering, University of Freiburg, Germany — [2]Materials, Physical and Chemical Sciences Center, Sandia National Laboratories, USA — [3]Institute for Applied Materials, Karlsruhe Institute of Technology, Germany — [4]Freiburg Materials Research Center, University of Freiburg, Germany — [5]Cluster of Excellence livMatS, University of Freiburg, Germany — [6]Department of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland

Surfaces in nature and engineering are often rough across many length scales, with self-affine scaling of heights. There is presently no unifying theory for the origin of roughness and self-affinity. One likely contributor is plastic deformation. In this work, the link between plastic deformation and self-affine roughness is investigated using molecular dynamics simulations. Three different materials are considered, single-crystal Au, the High Entropy Alloy $Ni_{36.67}Co_{30}Fe_{16.67}Ti_{16.67}$, and amorphous $Cu_{50}Zr_{50}$. Bi-axial compression of initially atomically flat surfaces of these materials is simulated. A self-affine topography emerges in all cases during plastic deformation, despite differences in composition, structure, and deformation mechanisms. Moreover, it is shown that non-affine displacements in the bulk scale self-affinely as well. The results indicate that self-affinity of plastic deformation is sufficient to explain the emergence of self-affine surface roughness.

MM 52: Materials for Energy Storage and Conversion - Ion Diffusion

Time: Thursday 10:15–11:30 Location: IFW D

MM 52.1 Thu 10:15 IFW D

measurement of Li mobility in lithium iron phosphate by APT at different field strength — •Ahmed Abdelkarim[1,2], Patrick Stender[1], and Guido Schmitz[1] — [1]Institute for Materials Science, Department for Material Physics, Stuttgart University, Stuttgart, Germany — [2]Spectroscopy Department, Physics Division, National Research Center (NRC), Cairo, Egypt

Lithium is considered to be the cornerstone of the energy storage in batteries. However, even for well- studied lithium insertion compounds such as Lithium Iron Phosphate (LFP) it is profoundly unclear how the ionic transport appears on a microscopic, even on atomic level scale. Ionic transport is 3 dimensionally studied by Atom Probe Tomography (APT). New unique insights into the mechanisms of Li movements have been provided. Through self-created fine columnar pathways, Li is pulled and Li enrichment/depletion regions are observed. It is demonstrated that this in-situ Li motion is dependent on the field strength of the measurements. In response to the applied fields, Li ions are undoubtedly redistributed. By mathematically modelling, the Li diffusion process is evaluated. Li diffusion in amorphous LFP shows a faster diffusion than crystalline over the whole laser range and is calculated to be a factor of about 100 faster at laser power 30 mW.

MM 52.2 Thu 10:30 IFW D

Atomistic analysis of migration properties of Li in $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ (LATP) solid electrolytes — Daniel Pfalzgraf[1,2], •Daniel Mutter[1], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, Germany

LATP [$Li_{1+x}Al_xTi_{2-x}(PO_4)_3$] is considered as one of the most promising ceramic materials to replace hazardous liquid electrolytes in all-solid state Li-ion batteries. This is mainly because of a three-dimensional structural diffusion network enabling fast transport of Li ions through well-defined channels. It has been observed that an Al ratio of $x = 0.3$ leads to the best performing compounds in terms of ionic conductivity. But a comprehensive understanding of this phenomenon is still missing. In this study, atomistic simulations based on density functional theory were performed to analyze the influence of Al substitution on Ti lattice sites on the migration behavior of Li. In LATP, the migration is dominated by a correlated mechanism involving three Li ions. In a systematic manner it is explored how different combinations of Al and Ti around the migration path change the energies of initial and final configurations as well as the energy barrier. "Al-like" and "Ti-like" behaviors can be identified, and the influence of the change of the LATP unit-cell volume with Al concentration is analyzed. We discuss the advancements and limitations of our approach in finding building blocks to describe quantitatively the Li migration in various arrangements of Al and Ti in LATP.

MM 52.3 Thu 10:45 IFW D

Investigating diffusion of lithium intercalated in graphite by a combination of multiscale modeling and NMR — •Cristina Grosu[1,2], Sandra Döpking[3], Chiara Panosetti[2], Simon Annies[2], Steffen Merz[1], Peter Jakes[1], Sebastian Matera[3], Josef Granwehr[1,4], and Christoph Scheurer[2] — [1]IEK-9, FZJ Jülich — [2]Chair for Theoretical Chemistry, TU Munich — [3]Institute for Mathematics, FU Berlin — [4]ITMC, RWTH Aachen

Lithium ion batteries play a key role in the implementation of fully sustainable electrical mobility. Long lifetime, fast recharging and safety are required for the acceptance of any battery powered vehicle. Graphite is still state of the art as negative electrode. Despite decades of investigation into the mechanism of lithium intercalation, the ion mobility and the underlying microscopic processes are still not fully understood, limiting progress in performance and lifetime prediction of a battery. In particular, improvements in fast charging of batteries mandates a deeper understanding of the lower states of charge (SoC), bellow or around 20%. We propose a combination of advanced NMR experiments, i.e spin alignment echo (SAE), with a theoretical multi scale modelling approach to investigate relevant phenomena such as lithium ion diffusion in graphite. Here, we present a novel multi-level accelerated first-principles kinetic Monte Carlo (1p-kMC) model to assess in detail the mobility at a low SoC, i.e LiC$_{108}$. In particular, an external potential is applied in order to mimic the driving force causing (dis)charge of the battery.

MM 52.4 Thu 11:00 IFW D

Measurements of lithium-ion conductivity at the grain level — •Peihua Huang, Patrick Uredat, Julian Zahnow, and Matthias T. Elm — Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen

Although lithium ion batteries (LIBs) have been commercialized since last century, there is still potential to improve the overall cell performance. One possibility for improvement is the optimization of the cathode of a LIB, where secondary particles of the active material are embedded in a conducting agent and binder material. The secondary particles themselves have a complex architecture consisting of primary particles in the nanoscale. As the microstructure has a strong influence on the transport properties, the characterization of the grain boundaries themselves is desirable. To study the transport across a grain boundary, thin layers of lithium cobalt oxide were deposited under various conditions by pulsed laser deposition. The films were subsequently annealed at various temperatures to facilitate grain growth to the micrometer range. Efforts on contacting single grain with microfabrication techniques have been made in order to study the lithium ion transport behavior at the grain level. For comparison, also the lithium ionic conductivity of the thin films has been measured.

MM 52.5 Thu 11:15 IFW D

First-principles study of magnesium transport in spinel chalcogenides — •Mohsen Sotoudeh[1], Manuel Dillenz[1], and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm — [2]Helmholtz Institute Ulm (HIU) for Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm

The ionic conductivity of spinel host materials has been studied using first-principles electronic structure calculations. The band-gap underestimation in density-functional theory has been corrected using the Hubbard U correction to the GGA Hamiltonian. In particular, we studied the influence of the metal distribution in the spinel materials and the ion concentration on the diffusion process. We carefully analyze the electronic and geometrical factors that determine the ion mobility and find an interesting correlation between ion concentration, lattice constant and the energetic ordering of magnesium insertion into tetrahedral and octahedral sites. Furthermore, we provide a mechanistic picture of the processes underlying Mg insertion and diffusion.

The work has been supported by the DFG through Germany's Excellence Cluster EXC-2154, project 422053626.

MM 53: Structural Materials (Steels, light-weight materials, high-temperature materials) - II

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

MM 53.1 Thu 11:45 BAR 205

Impact of Microstructural Engineered Steels on Micro Tensile Testing — •Jonas Kutschmann[1], Thomas Pretorius[2], Andreas Offergeld[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster — [2]thyssenkrupp Steel Europe AG, Kaiser-Wilhelm-Straße 100, D-47166 Duisburg

Mechanical properties of different microstructures of steels are characterized by micro tensile tests and compared to other mechanical testing methods. Out of the heavy plates, provided by thyssenkrupp, miniaturized specimens with a dog-bone shape contour were cut. The specimen dimensions have a constant gauge length of 4mm, the gauge cross-section has a dimension of around 0.5 x 0.5mm^2. The microstructure was modified by annealing treatment. The tensile test results are correlated to Vickers hardness measurements, average grain sizes by EBSD and macro tensile tests for the ultimate tensile strength.

All steels show a linear correlation between Vickers hardness and tensile strength. The Hall-Petch relation generally states that an increasing grain size leads to a lower yield strength. A critical grain size is reached when the average grain size gets close to the cross-section dimensions of the gauge. Possible deviations from the linear behavior of the Hall-Petch relation or a more pronounced decrease in yield strength in that regime are discussed.

MM 53.2 Thu 12:00 BAR 205

Alloying impact on phase stability in ZrAl$_3$ — •Dominik Gehringer[1], Florian Schmid[2], Stefan Pogatscher[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria — [2]Christian Doppler Laboratory for Advanced Aluminium Alloys, Chair of Nonferrous Metallurgy, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria

During homogenization, Al$_3$Zr-particles precipitate out of supersaturated Zr-alloyed aluminum alloys and serve for grain size stabilization via Zener drag and can contribute to an increased strength. Al$_3$Zr exhibits three different crystal structures, L1$_2$, D0$_{22}$ and D0$_{23}$ but only the L1$_2$ shows a favorable coherent interface with the aluminum matrix. Here we present an *ab initio* study of alloying impact on their stability by considering 16 doping elements. Three criteria were considered: site preference for the alloying elements, formation energies and stacking fault energies acting as a kinetic stabilization complementing the alloy design based solely on thermodynamics. In our contribution we will present the above described analysis in detail together with the suggested novel alloys. These predictions will be corroborated by our preliminary experimental results.

MM 53.3 Thu 12:15 BAR 205

Overcome the strength-ductility trade-off in steels by a novel short-range ordering strengthening concept — •Wenwen Song and Wolfgang Bleck — Steel Institute (IEHK), RWTH Aachen University

The enhancement of mechanical properties is of great importance for the modern steels design. By adopting the conventional strengthening mechanisms, strength can increase substantially, albeit at the expense of formability. In the present work, we propose a new pathway to overcome the strength-ductility trade-off by employing a novel short-range ordering (SRO) strengthening concept. The formation of the SRO in an Al-alloyed high-Mn steel was investigated by means of a combined method of ab initio calculations and various experimental approaches, e.g. in-situ high-energy synchrotron X-ray diffraction (SYXRD) and small angle neutron scattering (SANS). The results for the first time prove the presence of SRO in Fe-Mn-Al-C lightweight steels experimentally. The quantum mechanics based ab initio calculations provide an explanation of the SRO formation mechanism in Fe-Mn-Al-C steels. By an appropriate SRO formation control, the strength and ductility are enhanced either individually or simultaneously, which distinguishes the SRO strengthening concept from other conventional strengthening mechanisms. This SRO strengthening concept seems a promising strategy to overcome the strength-ductility trade-off and be further adopted in the current available continuous annealing production lines in the industry.

MM 53.4 Thu 12:30 BAR 205

Residual stresses in additively manufactured aluminum alloys — •Marc-André Nielsen[1], Emad Maadwad[1], Dieter Lott[1], Peter Staron[1], Sabine Bodner[2], Gerald Resch[3], Jozef Keckes[2], and Martin Müller[1] — [1]Institute of Material Research, Helmholtz-Zentrum Geesthacht, Germany — [2]Erich Schmid Institute, Montanuniversität Leoben, Austria — [3]Resch GmbH, Glojach, Austria

Additive manufacturing opened up new ways to produce parts with high geometric complexity, e.g. involving internal structures, leading to an increased interest in science and industry in the recent years. The mechanical behavior and load-bearing capacity of additively manufactured components, however, is still not really understood and subject of intensive research efforts. In particular, residual stresses (RS) play an important role e.g. for strength and fatigue properties. Therefore, RS distributions were investigated in various parts, fabricated from aluminium alloy powder (AlSi10Mg) using the Selective Laser Melting (SLM) technique. The produced samples consist of simple walls with a wall thickness of about 3 mm and different geometries involving, e.g., different edge curvatures. Residual stress fields were determined using high-energy X-ray diffraction. The diffraction studies were carried out in transmission geometry using a photon energy of 87.1 keV. The high energy allows to penetrate thicker samples. The influence of specimen geometry and production parameters on the RS state will be discussed and the RS in the investigated aluminum alloy will be compared with RS in 316L steel.

MM 53.5 Thu 12:45 BAR 205

Oxide Breakdown and Anodic Corrosion of Nickel Base Alloys — •Dominik Dworschak, Hsiu-Wei Cheng, and Markus Valtiner — TU Wien, Applied Physics, Vienna, AT

Transpassive and pitting corrosion behaviour of advanced materials such as nickel base alloys (NBAs) determines corrosion resistance in extreme environments. While Cr and Mo enhanced passivity is well characterized, mechanism of transpassive dissolution as well as pitting and subsequent repassivation, e.g. occurring during active corrosion or pickling, are unclear. Here, elemental dissolution currents during high anodic polarization and repassivation of a series of nickel base alloys were quantified using an ICP-MS flow cell. At high anodic potentials non-stoichiometric and decelerated dissolution rates depend on the selective segregation/dissolution of alloying elements and transpassive passive film formation. Oxide breakdown depends on the solution chemistry and local pH that establishes during dissolution. Samples after corrosion experiment were examined by X-ray photoelectron spectroscopy and high spatial resolution synchrotron X-ray fluorescence to revealing local nickel depletion, while chromium and iron were enriched in corroded areas. We also discuss the influence of ICP-MS cell design on the corrosion mechanism and hence on obtained results.

MM 53.6 Thu 13:00 BAR 205

Impact of paramagnetism on grain boundary energetics in FeMn — •Omkar Hegde, Tilmann Hickel, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

To understand the impact of the magnetic disorder on defect energetics and kinetics is, though conceptually and computationally challenging, important for designing Fe-based alloys. Since magnetic degrees of freedom change faster than atomic degrees of freedom in the high-temperature paramagnetic state, the atoms move according to an averaged force instead of instantaneous forces attained from each spin configuration.

Therefore, a new computationally efficient method based on spin-space averaging [1] (SSA) has been developed to handle magnetic disorder next to defects. First, we focus on the vacancies in FeMn system, for which we demonstrate that paramagnetism significantly affects atomic relaxations as well as diffusion barriers and thereby we explain why Mn diffusion shows a different temperature dependence than Fe-self diffusion in α-Fe. Next, we expand our method to extended defects and present the impact of paramagnetism on the grain boundary energetics of Mn in FeMn. Finally, we combine our results to propose a pathway for Mn segregation to grain boundaries.

[1] F Körmann, A Dick, B Grabowski, T Hickel, and J Neugebauer, Phys. Rev. B 85(12):125104, (2012).

MM 54: Topical Session: Interface-dominated phenomena - Crystallization and Microstructure Evolution

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

MM 54.1 Thu 11:45 IFW A

Atomistic investigation of phase boundary migration during solid-solid phase transformations in tungsten — •Yanyan Liang, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

The phase transformation between the topological close packed A15 and cubic BCC in the transition metal tungsten has recently incited attention, given the applications in microelectronics and spintronic devices where either BCC or A15 is favourable. The underlying atomistic processes greatly influence the kinetics of phase transformations, specifically the mobility and corresponding growth velocity of interfaces. At high temperatures, phase boundary migration can be captured by conventional molecular dynamics (MD) simulations. At moderate temperatures, however, enhanced sampling techniques are required due to the slow movement of the interface and corresponding extended timescales that need to be covered. We combine both, high-temperature MD and low-temperature enhanced sampling, to investigate phase boundary migration between A15 and BCC in W. From these simulations, we extract information concerning the growth mode, such as step nucleation and growth along the step edges or island formations. Furthermore, we investigate the influence of driving forces on interface migration at different mismatches between A15 and BCC. Together with the evaluation of energy barriers connected to the migration of the phase boundary, we provide novel insight into the atomistic mechanism and kinetics during the solid-solid phase transformation.

MM 54.2 Thu 12:00 IFW A

A study of texture controlled grain growth in thin films by 3D simulations — •Dana Zöllner and Igor Zlotnikov — B CUBE - Center for Molecular Bioengineering, TU Dresden, Tatzberg 41, 01307 Dresden

Historically, metallography used to be the purely two-dimensional characterization of the microstructure of materials by optical microscopy. The main problem: A 2D section through a complex three-dimensional entity gives us only a poor description of the true size and shape. Therefore, numerous attempts have been made to obtain full three-dimensional structural information experimentally. Nevertheless, in computer simulations as well as analytical theories coarsening in thin films is frequently treated as a two-dimensional process still today. In the present investigation, grain growth in thin films is modeled by three-dimensional Potts model simulations focusing on the influence of initial texture associated with the grain microstructure. Different initial crystallographic textures yield different spatial distributions of boundary mobilities in the grain boundary network leading to a diversity of coarsening kinetics.

MM 54.3 Thu 12:15 IFW A

Shedding light on polymorph selection and seeding mechanisms during crystal nucleation in metals — •Grisell Díaz Leines and Jutta Rogal — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University Bochum, Germany

Fundamental knowledge of the mechanism and the principles of polymorph selection during crystal nucleation is essential for the synthesis and control of materials with targeted properties. However, understanding the atomistic mechanism of crystallization poses a major challenge as many materials exhibit complex transitions with multiple steps, forming polymorphic structures. Here, we employ an advanced atomistic simulation method, transition path sampling, to investigate the formation mechanism of crystal clusters during homogenous and heterogeneous nucleation in metals. The analysis of the nucleation pathways in Ni shows that the formation of pre-ordered liquid regions with increased bond-orientational order facilitates the emergence of crystallites by decreasing the interfacial free energy. The pre-structured cloud acts as a precursor of crystallization and predetermines the polymorph selected. Furthermore, we explore how selected crystal seeds influence the polymorphic outcome and efficiency of the nucleation process in Ni. Our investigation reveals a novel mechanism of heterogeneous nucleation, demonstrating that the ability of small seeds to promote bond-orientational order fluctuations and template the formation of effective precursors in the liquid, is central to understand the enhancement of the nucleation probability and the selection of polymorphs during crystallization.

MM 54.4 Thu 12:30 IFW A

Impurity effect on microstructure homogeneity, recrystallization kinetics and mechanical properties in severe plastically deformed coppers — •Yao Jiang[1,2], Martin Peterlechner[2], Ruicong Gu[1], Jingtao Wang[1,3], and Gerhard Wilde[2,3] — [1]School of Materials Science and Engineering, Nanjing University of Science and Technology, 210094 Nanjing, P.R. China — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany — [3]Herbert Gleiter Institute of Nanoscience, Nanjing University of Science and Technology, 210094 Nanjing, P.R. China

Recrystallization and mechanical behavior of ultra-fine grained (UFG) copper prepared by equal channel angular pressing and nano-lamellar (NL) copper by ECAP with additional cryogenic rolling were investigated by comparing coppers with two different purity of 4N and 3N. Discontinuous nucleation and grain growth were observed to be uncorrelated to shear bands. The discontinuous recrystallization was considered to modify JMAK model and to quantify the microstructure inhomogeneity. Moreover, the thermal stability of the NL structure was comparable to the UFG structure, due to their similar activation energy for recrystallization. Superior strength and ductility was achieved in the partially recrystallized NL structural 3N copper. The present work proposed an effective strategy to tailor the nuclei sites and grain growth of the partial recrystallization by using localized shear bands and composition.

MM 55: Computational Materials Modelling - Magnetic Materials

Time: Thursday 11:45–13:00 Location: IFW B

MM 55.1 Thu 11:45 IFW B

A Phase Field Crystal Model for Magneto-Structural Interaction — •Rainer Backofen[1] and Axel Voigt[1,2] — [1]Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), 01062 Dresden, Germany

Phase field crystal (PFC) modeling is based on a free energy for a smoothed particle density. The energy is minimized by a smoothed particle density, that has the basic symmetry of the crystal. Thus, defects, elasticity and plasticity is natural included.

In order to include magneto-structural interaction, local magnetization is coupled with a structural PFC model [1,2]. We will discuss the coupling and show how to control the magnetic properties of the model. This extended PFC model is used to study the impact of external magnetic fields on grain boundary movement and on coarsening in thin films [2].

[1] N.Faghihi et al. PRE 88, 032407 (2013).

[2] R. Backofen et al. PRL 122, 126103 (2019).

MM 55.2 Thu 12:00 IFW B

Modeling of magnetodyanmics in endohedral-fullerene-based molecular magnets — •Stanislav Avdosheno and Alexey Popov — Leibniz Institute for Solid State and Materials Research (IFW), D-01069 Dresden, Germany

Systems dynamics is the merit of the system complexity. In the single molecular magnets(SMMs) research, there are many aspects that make SMMs very complex. Well before any magnetic measurements begin, the molecular dynamics control the structures and order of SMMs in bulks or on surfaces. In the end, this impacts strongly the magnetic feedback of the whole system. Through the magnetic measurement itself, the magnetic states evolve accordingly to the quantum equation of motion. The quantum dynamic is coupled strongly with local atomic motions with substantial effects on magnetic stability.

In this contribution, we report such dynamical effects in the application to the endohedral-fullerene-based molecular magnets. We showed how the molecular dynamics modeling helps to understand which structural elements to expect on the metallic and dielectric surfaces. Having used ab initio methods, we have been able to derive the fundamental properties of Ln containing endohedral-fullerene molecular magnets. This helped to rationalize and to have a deep understanding of magnetic relaxation in these systems. Finally, we also introduced a simple model, based on the existing open quantum systems theories, able to predict the spin relaxation dynamics with implicit and explicit phonons in the system Hamiltonian.

MM 55.3 Thu 12:15 IFW B

An advanced method for computing the intrinsic spin Hall conductivity from first principles — •Minsu Ghim, Ji Hoon Ryoo, and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea, Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea, Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Spin Hall effect plays a key role in spintronics. It is widely accepted that the spin Hall conductivity can be categorized into three different contributions: skew-scattering, side-jump, and intrinsic. Recently, methods for computing the intrinsic spin Hall conductivity from first principles using the maximally-localized Wannier functions have been reported [1,2]. In this talk, we present technical improvements of the original method [2] in terms of computational efficiency.

[1] J. Qiao, J. Zhou, Z. Yuan, and W. Zhao, Phys. Rev. B 98, 214402 (2018) [2] J.-H. Ryoo, C.-H. Park, and I. Souza, Phys. Rev. B 99, 235113 (2019)

MM 55.4 Thu 12:30 IFW B

A three-order-parameter, bistable, magnetoelectric multiferroic metal — Andrea Urru[1,2], Francesco Ricci[3], Alessio Filippetti[1], Jorge Iniguez[4], and •Vincenzo Fiorentini[1] — [1]Dip Fisica, Uni Cagliari, Italy — [2]SISSA, Trieste, Italy — [3]University of Louvain-la-neuve, Belgium — [4]LIST, Luxembourg

Using first-principles calculations we predict that the layered-perovskite metal Bi5Mn5O17 is a ferromagnet, a (switchable) ferroelectric, and a ferrotoroid, and has two energy-degenerate ground states with distinct polar, magnetic, and toroidic axes. In both states, the three vector order parameters (polarization, magnetization, ferrotoroidic moment) are mutually orthogonal, so they can be rotated globally by switching between ground states. Importantly, Bi5Mn5O17 is expected to be thermodynamically stable in O-rich growth conditions.

MM 55.5 Thu 12:45 IFW B

Magnetic and Electronic properties of Mn2Au: A Novel spintronic compound — •Sunil Wilfred DSouza[1], Hans-Joachim Elmers[2], Satya Prakash Bommanaboyena[2], Martin Jourdan[2], and Jan Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Univerzitní 8, CZ-306 14 Pilsen, Czech Republic. — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany

The band structure of bulk Mn2Au has been investigated by first-principles density-functional theory calculations based on the Green*s function technique. The total density of state reveals contributions mainly from the Au5d and Mn3d states with rigid local moments on the Mn sites. The existence of significant out-of-plane magnetic anisotropy combined with the large strength of short range antiferromagnetic exchange interactions between Mn atoms located at two different Wyckoff positions results in the stabilization of the antiferromagnetic ground state. Two dimensional plots of constant energy surfaces in the Γ-X-Σ plane of the Brillouin zone exhibits a four-fold to two-fold symmetry breaking as a function of the binding energy at 0.00 eV and 0.25 eV below the Fermi surface. We find that such a symmetry breaking in Mn2Au is arising due to the degeneration of the electronic bands in the presence of external magnetic field indicating a strong spin-orbit coupling interaction. Our results describes the tuning of the magnetic and electronic properties of Mn2Au for spintronic applications.

MM 56: Materials for Energy Storage and Conversion - Intercalation

Time: Thursday 11:45–13:00 Location: IFW D

MM 56.1 Thu 11:45 IFW D

Modulation of the optical properties of LixCo2O via Li-ion transport — •Sanaz Banifarsi[1], Yug Joshi[2], Robert Lawitzki[3], and Guido Schmitz[4] — [1]Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Heisenbergstrasse 3, 70569 Stuttgart, Germany — [3]Heisenbergstrasse 3, 70569 Stuttgart, Germany — [4]Heisenbergstrasse 3, 70569 Stuttgart, Germany

Modulation of the optical properties of LixCo2O via Li-ion transport

Sanaz Banifarsi, Yug Joshi, Robert Lawitzki, Guido Schmitz

University of Stuttgart, Institute for Materials Science, Chair of Materials Physics.

Heisenbergstrasse 3, 70569 Stuttgart, Germany

Previous studies reveal that the electronic structure of Lithium cobalt oxide (LixCoO2, LCO) undergoes severe change upon lithium de-/intercalation. The present study probes this behavior by combining electrochemistry with Vis-NIR spectroscopy of the LCO during the battery cycling. To this aim, thin films of LCO serving as an active material were deposited on the platinum metallization (on oxidized silicon wafer, acting as current collector as well as a reflector), by ion beam sputtering. The structure of the active material is investigated by X-ray diffraction and transmission electron microscopy. The refractive index, derived from the Clausius-Mossotti dispersion equation, as a function of wavelength evolves upon lithium de-/intercalation. The study attempts at linking this evolution of the dispersion curves to the underlying electronic structure of the LCO. In addition, in situ electrochemical measurement proves electrochromic reversibility.

MM 56.2 Thu 12:00 IFW D

Laser-assisted atom probe tomography (APT) study on the lithiation behavior in the conversion reaction of CuO as an anode in lithium ion battery — •Jianshu Zheng, Patrick Stender, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Heisenbergstr. 3, D-70569 Stuttgart, Germany

The lithiation behavior in conversion reaction of CuO as an anode in lithium ion battery is investigated by the laser-assisted atom probe tomography (APT). For this purpose, the CuO thin film is firstly prepared by ion beam sputtering, then lithiated to various conversion states via electrochemical techniques, afterwards lifted out and glued onto Tungsten post, and further shaped into sharp tip with diameter smaller than 100 nm by focus ion beam, before it is finally measured in laser-assisted APT. The following reconstruction on the resultant data provides the 3D coordinates of atoms in real space, enabling us to view the distribution of atoms and concentration profiles within certain volumes. Three conversion states in the first cycle of CuO are studied, where in the initial, intermediate, and fully conversion states, lithium clusters, a mixed compound CuOLix (0<x<2), and nanometer-scaled metallic Cu particles in Li2O matrix are observed, respectively. With the advantage of APT, the size distribution of Cu particles and the concentration profile across the Cu/Li2O interface are obtained, revealing the structure and concentration evolution of Cu particles in Li2O matrix. Based on the above results, a model on the diffusion pathway and kinetics of lithium ions is created.

MM 56.3 Thu 12:15 IFW D

Quantifying the intercalation process in graphite based anode materials using DFT — •Holger Euchner[1] and Axel Gross[1,2] — [1]Helmholtz Institute Ulm for Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm — [2]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm

Carbon derivatives such as hard carbon are considered as anode materials for Li-ion and particularly post Li-ion technology. Despite its importance, the underlying storage mechanism in the different types of carbon based anodes and for different alkali metal cations is still debated and clear characterization strategies are missing.

In this contribution, we present lattice dynamics and band structure calculations for different stages of alkali metal intercalation in graphitic model structures as obtained from periodic denisty functional theory. An interpretation of these results with respect to Raman and double resonance Raman scattering – focussing on the G-band and D-band excitations – suggests D- and G-band as sensitive descriptors of the intercalation process [1]. Consequently, these insights may be used for distinguishing the exact insertion mechanism for different alkaline metals in carbon based materials.

[1] M. Anji Reddy, M. Helen, A. Groß, M. Fichtner, H. Euchner, ACS Energy Lett. **3**, 2851 (2018).

MM 56.4 Thu 12:30 IFW D

A new hop: a DFTB model for Li diffusion in low-SOC graphite anodes. — •Chiara Panosetti[1], Simon Annies[1], Cristina Grosu[1,2], Maria Voronenko[1], and Christoph Scheurer[1] — [1]T. U. München — [2]Forschungszentrum Jülich

Despite having been employed in consumer electronics for decades, Li-graphite anodes are not yet understood enough to *e.g.* upscale usage towards automotive applications. Many mechanisms involved in charging/discharging, ageing, and other key aspects, were never grasped in detail. Part of this difficulty is due to a structural complexity emerging particularly at low states of charge (SOC), which complicates both the interpretation of experiments and the computational modelling. From a computational standpoint, targeted system sizes compatible with the SOC range of interest are inaccessible to first-principles calculations, yet require first-principles treatment of key effects such as dispersion and long-range electrostatics. Density-Functional Tight Binding (DFTB), a semi-empirical approximation to DFT, offers a high-quality trade-off between accuracy and speed. With our recently developed parametrization [1], we are able for the first time to resolve the full Potential Energy Surface (PES) of Li motion in stage-I and stage-II LiC$_{108}$ (SOC 5%). The PES contains information that enables us to implement, and hereby discuss, both kinetic Monte Carlo (kMC) models of Li-ion mobility in the graphite host, and free-energy sampling which ultimately yields the computed voltage profile of the anode.

[1] C. Panosetti *et al.*, arXiv:1904.13351 (2019).

MM 56.5 Thu 12:45 IFW D

The Electrostatic GAP: Machine-Learning Potentials for Battery Materials — •Carsten Staacke[1], Christoph Scheurer[1], Johannes Margraf[1], Gabor Csanyi[2], and Karsten Reuter[1] — [1]Chair of Theoretical Chemistry, TUM, Germany — [2]Engineering Department, Cambridge University, UK

All-solid-state Li-ion batteries promise gains in safety and durability by combining high Li-ion conductivity and mechanical ductility. In this respect, solid-state electrolytes (SSE) such as the Li$_7$P$_3$S$_{11}$ glass-ceramic have gained much attention.[1] From a modelling perspective, describing ionic conductivity and the role of crystalline/amorphous interfaces in such SSEs requires an accurate and efficient description of covalent and electrostatic interactions. To this end, we have combined short-ranged machine-learning potentials based on the Gaussian Approximation Potential (GAP)[2] approach with a classical electrostatic model in the long-range. We will present a first-principles validation of both, pure GAP potential and the new electrostatic GAP for the LPS SSE. In particular, the role of Coulomb interactions in SSE simulations will be shown and evaluated.

[1] A. Hayashi, A. Sakuda, M. Tatsumisago, *Front. Energy Res.,* ***2016****, 4, 25* [2] A. P. Bartók, M. C. Payne, R. Kondor, G. Csányi *Phys. Rev. Lett.,* ***2010****, 104, 136403*

MM 57: Invited talk Greiner

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

Invited Talk MM 57.1 Thu 15:00 BAR 205

Deformation mechanisms in metals under a tribological load — •Christian Greiner — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Karlsruhe, Germany

About twenty percent of the world's primary energy consumption is spend to overcome friction and wear. In 1950, Bowden and Tabor pointed out that in metallic tribological contacts, the majority of the dissipated energy is dissipated to change the contacting materials' microstructures. This - in part - explains why most metals show a highly dynamic subsurface microstructure under the shear load imposed by a sliding contact. In order to understand these processes, the elementary mechanisms accommodating the shear strain and acting in the material need to be revealed and understood. In this presentation, three examples of research avenues following this hypothesis will be given. During the very early stages of sliding, dislocations show an interesting self-organization phenomenon. The evolution of such structures will be presented as well as similarities and difference between copper and the high entropy alloy (HEA) CoCrFeMnNi be pointed out. Finally, we will focus our attention on tribo-chemically activated oxidation processes and what role crystal defects have to play in this context.

MM 58: Topical Session: Data Driven Materials Science - Machine Learning for Materials Characterization (joint session MM/CPP)

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

Topical Talk MM 58.1 Thu 15:45 BAR 205

Machine learning tools in analyticat transmission electron microscopy — •Cécile Hébert and Hui Chen — LSME, Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Analytical scanning transmission electron microscopy probes the chemistry of the investigated sample by recording spectral information as a function of electron probe position. The acquired spectra can consist of X-Ray photons emitted by the sample after the incoming electron probe has excited it (EDX) and/or an analysis of the energy lost by the incoming electron when it excites the sample (EELS). Both EELS and EDX spectra can be recorded on a scanned area consisting of 1000x1000 pixels of even more, leading to a so called *hyperspectral datacube* of up to several 10^6 spectra. Such a vast amount of data calls for machine learning tools belonging to the family of multivariate statistical analysis (MSA). Such methods have been implemented and used since the mid-ninties, however, there are still many challenges related to their application. MSA methods are very sensitive to detector artifacts, they deliver components, which do not necessarily bear a physical meaning, they might discard small and very localized signal, etc. In this presentation, I will review the use of unsupervised machine learning in analytical TEM, and present some new results based on a dictionary learning approach where we implement knowledge we have about the shape of the spectral components.

MM 58.2 Thu 16:15 BAR 205

Automatic semantic segmentation of Scanning Transmission Electron Microscopy (STEM) images using an unsupervised machine learning approach — •Ning Wang, Christoph Freysoldt, Christian Liebscher, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

The recent substantial advance of machine learning provides us with a rich toolbox to successfully address problems in materials science. Here we present an unsupervised machine learning approach for automatic semantic segmentation of STEM images. We propose a robust descriptor, the local correlation map, for characterization of the local periodicity, which is then fed into an unsupervised clustering algorithm in order to segment the STEM images into different crystalline regions. The semantic segmentation works as an initial step for further data analysis, such as image denoising, extraction of lattice vectors and so on. As a proof of concept, we apply our approach to STEM images of Cu grain boundaries, Ni stacking faults and twin boundaries, and Fe2Nb phase boundaries, and observe very good robustness and resolution.

MM 58.3 Thu 16:30 BAR 205

Bayesian models and machine-learning for NMR crystal structure determinations — •Edgar Albert Engel[1], Andrea Anelli[2], Albert Hofstetter[3], Federico Maria Paruzzo[3], Lyndon Emsley[3], and Michele Ceriotti[2] — [1]TCM, University of Cambridge, United Kingdom — [2]COSMO, Ecole Polytechnique Federale de Lausanne, Switzerland — [3]LRM, Ecole Polytechnique Federale de Lausanne, Switzerland

NMR spectroscopy is a key tool for determining the atomic structure of powdered and amorphous solids, which usually proceeds by finding the best match between experimentally observed NMR chemical shifts and those of candidate structures. However, the reliability of structure determinations depends on the errors in the predicted shifts. I will demonstrate how a Bayesian approach based on knowledge of the typical errors, coupled to visualisations of the similarity of the candidate structures, allows to quantify and understand the resultant confidence in the identifications of the experimental structure [1]. The applications highlight that using self-consistently determined uncertainties instead of commonly used global estimates make it possible to use 13C shifts to improve the accuracy of structure determinations. I will further outline how a machine-learning approach including uncertainty estimation [1,2] ties in with the above structure determination framework and that it can provide a surrogate for costly or even outright unfeasible first-principles predictions of NMR shifts.

[1] E. A. Engel et al., Phys. Chem. Chem. Phys., 21, 23385 (2019) [2] F. M. Paruzzo et al., Nature Comm., 9, 4501 (2018)

MM 58.4 Thu 16:45 BAR 205

Teaching machines to learn dynamics in NMR observables — •Arobendo Mondal, Karsten Reuter, and Christoph Scheurer — Chair for Theoretical Chemistry, TU Munich, Germany

NMR is a powerful tool for studying the structural and electronic properties of molecules and solids. However, the interpretation of NMR spectra for large systems is often challenging as a result of the free or constrained dynamics of the ligands attached to the NMR active nucleus. Computed NMR parameters can aid in the interpretation. Their accuracy depends on the level of method used, with the high computational cost of highly accurate first-principles calculations quickly limiting the tractable system sizes and number of such computations.

In this respect, emerging machine learning approaches are an appealing option. The key challenge here is an efficient data representation, as NMR parameters depend strongly on their local chemical environment with often non-negligible effects of the second and third coordination sphere. To this end, we use a combination of multiple SOAP descriptors[1] to learn NMR parameters for the Antamanide peptide molecule from quantum chemical data computed on a small subset of a long 90 ns molecular dynamics trajectory. The trained model is found to predict NMR parameters within DFT accuracy for 90,000 snapshots from this trajectory that were not contained in the training data.

[1] Phy. Rev. B, **2013**, *87*, 184115

MM 58.5 Thu 17:00 BAR 205

Automatic Identification of Crystallographic Interfaces from Scanning Transmission Electron Microscopy Data by Artificial Intelligence — •Byung Chul Yeo[1], Christian H. Liebscher[2], Matthias Scheffler[1], and Luca Ghiringhelli[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Characterizing crystallographic interfaces in synthetic nanomaterials is an important step for the design of novel materials, e.g., catalysts, gas sensors, etc. In principle, trained materials scientists can assign interface structures of materials by looking at high-resolution imaging and diffraction data obtained by aberration-corrected scanning transmission electron microscopy (STEM). However, the high-acquisition rates in STEM pose a challenge to a purely human-based identification of interfaces or defects. As of today, STEM datasets are being massively accumulated, but they cannot be fully exploited due to the lack of automatic analysis tools. Here, we present a newly developed artificial-intelligence tool for accurately extracting the key features of (poly)crystalline materials, i.e., crystal-structure prototype, lattice constant, and (relative) orientation from atomic-resolution STEM images. The tool is based on a convolutional neural network and operates on both high-angle annular dark-field (HAADF) and convergent beam electron diffraction (CBED) images. The network is trained on 13 200 simulated STEM images, including structures distorted by thermal noise, and our model achieves excellent predictive performance for automatically identifying crystal structure and lattice misorientations.

MM 59: Computational Materials Modelling - Potentials

Time: Thursday 15:45–17:15 Location: IFW A

MM 59.1 Thu 15:45 IFW A

A platform for the validation of interatomic potentials — •Yury Lysogorskiy, Thomas Hammerschmidt, and Ralf Drautz — AMS, ICAMS, Ruhr University Bochum, Bochum, Germany

Interatomic potentials (IPs) are widely used in computational materials science, in particular for simulations that are too computationally expensive for density functional theory (DFT). A large number of IPs is available for a wide range of chemical elements and their mixtures. Most IPs have a limited application range and often there is very limited information available regarding their performance for specific simulations. We performed extensive tests for the majority of the available potentials from the OpenKIM and NIST repositories as well as from other sources. In this talk we present the online platform **atomistictools.org** for the validation of IPs. The platform offers efficient visualization of various tests and ranking of the IPs. Predictions of the IPs are compared to reference data (DFT and experiment, if available). The platform further provides direct access to the tests, reference data and protocols in order to that potential developers can integrate this into their workflow for parameterizing novel potentials.

MM 59.2 Thu 16:00 IFW A

Machine-learned density-functional tight-binding: Enabling high-quality electronic structure calculations on systems too large for DFT — •Simon Anniés, Chiara Panosetti, Christoph Scheurer, and Karsten Reuter — Technical University Munich

Density-Functional Theory (DFT) has been one of the go-to methods for electronic structure calculations for several decades. Nevertheless, inherent scaling properties and/or large prefactors for linear-scaling implementations still limit its usability for larger systems or extensive sampling.

Density-Functional Tight-Binding (DFTB), a semi-empirical approximation to DFT, is an alternative that - as opposed to forcefields - retains access to electronic structure properties while providing a speed-up of roughly three orders of magnitude. The trade-off is a two-part parametrization process. The numerical parameters of the electronic part are optimized by comparing with DFT bandstructures, the repulsion potential by forcematching against representative training sets from high-level electronic structure methods.

In our work, we apply a machine learning approach, making use of Gaussian Process Regression (GPR), in order to greatly increase the adaptability of the repulsion potential. By embracing a purely data-driven methodology, this overcomes the limitations of previously employed rigid functional forms. We demonstrate the superior transferability of this approach in the application to lithium-intercalated graphite as prevalent anode material of commercial lithium-ion batteries.

MM 59.3 Thu 16:15 IFW A

Machine Learning Augmented Density Functional Tight Binding Theory — •Adam McSloy[1], Benjamin Hourahine[2], David Yaron[3], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick — [2]Department of Physics, University of Strathclyde — [3]Department of Chemistry, Carnegie Mellon University

Density functional tight binding theory (DFTB) is a cost-effective electronic structure method which excels at reaching the size and time scales normally off limits to Density Functional Theory and other electronic structure methods. However, the derivation of parameter sets for systems beyond simple semiconductors and organic molecules is a non-trivial task. Here, we present a deep machine learning framework to construct DFTB parameter sets and apply it to construct a new parameter set for hybrid organic-metallic materials. Furthermore, we show that machine learning offers a way to extend the DFTB method beyond the two-centre approximation, which enables a more accurate treatment of reactive chemistry and non-equilibrium dynamics.

MM 59.4 Thu 16:30 IFW A

Towards transferable parametrization of Density-Functional Tight-Binding with machine learning — •Leonardo Medrano Sandonas, Martin Stöhr, and Alexandre Tkatchenko — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg.

Machine learning (ML) has been proven to be an extremely valuable tool for simulations with ab initio accuracy at the computational cost between classical interatomic potentials and density-functional approximations. Similar efficiency can only be achieved by semi-empirical methods, such as density-functional tight-binding (DFTB). One of the limiting factors in terms of the accuracy and transferability of DFTB parametrizations is the so-called repulsive potential, which plays a considerable role for the prediction of energetic, structural, and dynamical properties. Few attempts of using ML-techniques to address this issue have been proposed recently [1] but, up to now, evidence of transferability and scalability is still scarce. Using the QM7-X database of small organic molecules, we demonstrate that the DFTB repulsive energy can be effectively learned by means of ML-approaches including neural networks and kernel ridge regression. We further show how the resulting DFTB+ML model can also be used for more complex systems like molecular dimers and crystals, and modeling techniques like (global) structure search or vibrational analysis. DFTB+ML thus opens a route to the simultaneous access to reliable electronic and structural/dynamical properties of diverse molecular systems. [1] J. J. Kranz et al., J. Chem. Theory Comput., 14, 2341-2352, (2018).

MM 59.5 Thu 16:45 IFW A

Anharmonic phonons at elevated temperatures in Al — •Michael Leitner[1] and Albert Glensk[2,3] — [1]Technische Universität München, 85748 Garching, Germany — [2]Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland — [3]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

The importance of anharmonicity for describing fundamental materials properties, starting from finite heat conductivity due to phonon-phonon scattering, can hardly be overemphasized. For crystalline matter, the principal microscopic gauge is constituted by the broadening in energy of the phonon dispersions, corresponding to q-dependent phonon lifetimes.

Here the case of elemental Al at temperatures up to the melting point will be considered. Experimental data obtained by inelastic neutron scattering will be compared to calculations of q-dependent line broadenings on the basis of density-functional theory. The agreement with spectra computed by ab initio molecular dynamics is satisfactory, while the standard approach of perturbation theory gives significant discrepancies. Finally, an analysis of the atomic interaction constants will show how numerically efficient phenomenological potentials can be constructed that allow to compute anharmonic properties beyond the limitations of perturbation theory at very small computational effort.

A. Glensk et al., to be published in Phys. Rev. Lett. (2019)

MM 59.6 Thu 17:00 IFW A

Comparative Study of Interatomic Potentials for Atomistic Simulations of Sintering of α-Alumina — •Arun Prakash, Shyamal Roy, and Stefan Sandfeld — Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg

Crystalline alumina (α-alumina) with a corundum structure exhibits excellent material properties and is usually processed via sintering. At the nanoscale, sintering and the properties of the sintered material are often determined by atomic scale processes. Atomistic simulations are ideally suited to study and gain valuable insights into such fundamental processes, but their accuracy is, however, determined by the interatomic potential used.

In this work, we perform a systematic study of different interatomic potentials for the sintering of α-Al$_2$O$_3$ via atomistic simulations. The compared potentials are: Vashishta, Buckingham/Matsui type, Born-Mayer-Huggins type and Charge Transfer Ionic + EAM (CTI+EAM). We first compare fundamental properties like e.g. surface energies, elastic constants etc. via molecular statics, and then simulate sintering of thin slab like structures via molecular dynamics. We analyze the simulations in terms of both global quantities and local mechanisms. The differences in the sintering simulations are correlated to the fundamental properties of the individual potentials. Finally, we discuss the consequences of the usage of such potentials for atomistic simulations

MM 60: Mechanical Properties: Plasticity, fracture, fatigue, wear - I

Time: Thursday 15:45–17:15 Location: IFW B

MM 60.1 Thu 15:45 IFW B

Origins of Strength and Plasticity of the precious metal based high entropy alloy AuCuNiPdPt — •Felix Thiel[1,5], Daniel Utt[2], Dirk Seifert[1], David Geissler[1], Alexander Kauffmann[3], Sascha Seils[3], Martin Heilmaier[3], Karsten Albe[2], Mykhaylo Motylenko[4], David Rafaja[4], Jens Freudenberger[1,4], and Kornelius Nielsch[1,5] — [1]Leibniz-IFW Dresden — [2]TU Darmstadt — [3]Karlsruhe Institut für Technologie — [4]TU Bergakademie Freiberg — [5]TU Dresden

The precious metal based High-Entropy Alloy (HEA) AuCuNiPdPt crystallises in a fcc structure and is single phase without chemical ordering. This HEA shows extended malleability during cold work up to a logarithmic deformation degree of $\varphi = 2.42$. The yield strength ranges from 820 MPa in the recrystallised state to 1170 MPa when strain hardened by cold working. The high strength in the recrystallised state is evaluated and found to originate predominantly upon solid solution strengthening. The work hardening behaviour is traced back to a steep increase in dislocation density as well as in deformation twinning. The microstructure and the mechanical properties of AuCuNiPdPt are assessed in detail.

MM 60.2 Thu 16:00 IFW B

Variation of mechanical strength with composition in the Cantor alloy system: Experiments and modeling — •Daniel Utt[1], Tom Keil[2], Alexander Stukowski[1], Enrico Bruder[2], Karsten Albe[1], and Karsten Durst[2] — [1]Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — [2]Fachgebiet Physikalische Metallkunde, Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

We investigate the concentration dependent mechanical properties of the Cantor high-entropy alloy (HEA) system over a wide concentration range and aim to understand the influence of the different chemical elements on the alloy's strength and phase stability. The investigated samples are the different subsystems of the HEA, where one element of the alloy is enriched, while the others are decreased using diffusion couple samples of the HEA and each of its constituents.

The concentration gradient in the interdiffusion zone allows us to determine the concentration dependent phase stability and solid solution strengthening (SSS). Here, the phase stability is measured using electron backscatter diffraction and compared to THERMO-CALC predictions. The strength of the alloy is determined by nanoindentation hardness measurements. The resulting SSS is described using two models. The Labusch model does not have predictive power but it reveals that Cr is the most potent strengthener. The Varvenne model describes the concentration dependent SSS in the Cantor alloy system well for all investigated diffusion couples.

MM 60.3 Thu 16:15 IFW B

Exploring slip across Laves phase interface in magnesium alloy — •Julien Guénolé[1,2], Muhammad Zubair[1], and Sandra Korte-Kerzel[1] — [1]Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, Germany — [2]LEM3 - CNRS, Metz, France

The mechanical behaviour of Mg-Al alloys can be largely improved by the formation of an intermetallic Laves phase skeleton, in particular the creep strength. Recent nanomechanical studies revealed plasticity by dislocation glide in the Mg2Ca Laves phase, even at room temperature. As strengthening skeleton, this phase remains however brittle at low temperature. In this work, we present experimental evidences of slip transfer from the Mg matrix to the Mg2Ca skeleton at room temperature. We further explore the associated mechanisms by means of atomistic simulations and identify two type of slip transfer depending on the crystallographic orientation: a direct and an indirect slip transfer.

MM 60.4 Thu 16:30 IFW B

Uncovering Fundamental Subsurface Deformation Mechanisms in High-Purity Copper Induced by Sliding — •C. Haug[1,2], F. Ruebeling[1,2], A. Kashiwar[3,4], P. Gumbsch[1,3,5], C. Kübel[3,4,6], and C. Greiner[1,2] — [1]Karlsruhe Institute of Technology (KIT), IAM, Karlsruhe, Germany — [2]KIT IAM-CMS MicroTribology Center — [3]KIT, INT — [4]Department of Materials and Earth Sciences, Technical University of Darmstadt (TUD), Darmstadt, Germany — [5]Fraunhofer IWM, Freiburg, Germany — [6]KIT, KNMF

Friction and wear in mechanical systems greatly contribute to global energy consumption. Fundamental studies of the mechanisms governing dislocation mediated plastic deformation and friction at metal sliding interfaces may greatly help expedite the development of materials tailored for low friction and little wear. The present work therefore investigates the microstructural changes induced by sliding in the vicinity of a twin boundary in high-purity copper. The formation of two distinct horizontal line features (dislocation trace lines, DTL) parallel to the sliding interface is observed and their interaction with the twin boundary studied by means of automated crystal orientation mapping (ACOM). Utilizing the twin boundary as a marker, three concurrent fundamental deformation mechanisms are discerned: First, a simple shear process affecting the immediate subsurface area. Second, a localized shear process at the lower DTL. Third, a crystal rotation of the areas between the sliding interface and both DTLs. The three processes are found to exhibit a strong compatibility. Their identification is decisive for guiding future experimental and modeling efforts.

MM 60.5 Thu 16:45 IFW B

Size effect in bi-crystalline Cu micropillars with a coherent twin boundary — •Reza Hosseinabadi, Gerhard Dehm, and Christoph Kirchlechner — Max-Planck-Institut für Eisenforschung GmbH

It was recently shown by micropillar compression that the stress for ideal dislocation slip transmission through a Coherent Twin Boundary (CTB) is similar to the stress required for dislocation cross-slip. The difference in shear stress of a single and bi-crystalline micropillar (Δ*2%) can be as low as 7 MPa. A double-hump dislocation shape was proposed to explain the unexpectedly low difference, where an additional curvature of dislocations in bi-crystalline micropillars is necessary to form a perfect screw dislocation required for the cross-slip-like slip transmission.

Aim of this study is to study the size scaling of CTB containing micropillars to validate or revise the double-hump theory. We employ Focused Ion Beam (FIB) machining to mill more than 120 micron-sized single and bi-crystalline pillars with a single vertical $\Sigma3(111)$ CTB. Subsequently, in situ microcompression experiments inside a scanning electron microscope (SEM) as well as post-mortem imaging using SEM were performed.

Bi-crystalline pillars follow the same size scaling laws as typically observed in micro-pillars, i.e. smaller are substantially stronger. Furthermore, Δ*2% tends to increase with reduced pillar diameters. This effect can be explained by the double-hump theory and will be quantitatively compared to model predictions.

MM 60.6 Thu 17:00 IFW B

How to optimize strength and conductivity in metallization layers by alloying? — •Viswanadh Gowtham Arigela[1], Tobias Oellers[2], Alfred Ludwig[2], Christoph Kirchlechner[1], and Gerhard Dehm[1] — [1]Structure and Nano-/ Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Dusseldorf, Germany — [2]Institute of Materials, Ruhr-Universität Bochum, Bochum, Germany

The current trend of ever harsher environments and power densities in microelectronic applications brings the need of enhanced thermo-mechanical and electrical properties in metallization layers. It is of particular interest to develop copper alloys with improved strength at service temperature, which can be up to 400°C. Consequently, mechanical characterization of these systems at their service conditions at the micrometer length scale is required. We have used combinatorial approaches to synthesize binary Cu-Ag and Cu-Zr alloys with the aim of enhancing the mechanical properties. The specimens were fabricated from thin-film material libraries using photolithography. The mechanical properties of the alloys were investigated at temperature of up to 400°C using microtensile specimens. Finally, the deformation mechanisms were investigated by scanning electron and transmission electron microscopy. In the talk we will show a substantial improvement of the thin film performance of the alloys. Furthermore, we discuss the underlying strengthening mechanisms. Based on the results we will discuss how alloys with an optimized combination of strength and conductivity can be realized for microelectronic applications.

MM 61: Nanomaterials - I

Time: Thursday 15:45–17:15 Location: IFW D

MM 61.1 Thu 15:45 IFW D

Nanoporous Copper-Nickel – Macroscopic bodies of a strong and deformable nanoporous base metal by dealloying — •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

Owing to their very large surface area to volume ratio, nanoporous metals made by dealloying in aqueous solutions promise significant functionalization. Potential applications arise as actuators, sensors, catalysts or structural materials with tunable mechanical properties. An obvious require-ment for a materials competitive ability in these fields is affordability. In addition, deformability is required to avoid premature failure upon exposure to stress concentrations or to designed mechanical load. So far, macroscopic samples of nanoporous metals with a high surface area and deformability have been limited to precious, and thereby costly, metals such as Au, Pd and Pt.

Here we present nanoporous Copper-Nickel (npCN), a nanoporous base metal that can be made in macroscopic dimensions (> several mm in size) and shows significant deformability. Fabricated through dealloying in aqueous media, npCN exhibits a uniform, bicontinous network structure with feature sizes that can be controlled from 13 to 40 nm through thermal annealing. Continuous com-pression tests find ductile deformation behavior accompanied with a high strength compared to other nanoporous base metals as well as macroporous Cu- and Ni-foams with similar solid fraction.

MM 61.2 Thu 16:00 IFW D

Elastic and plastic behavior of nanoporous gold under applied electrochemical potential — •Yijuan Wu[1], Jürgen Markmann[1,2], and Erica Lilleodden[1,3] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

The elastic and plastic behavior of nanoporous gold (NPG) under electrochemical potential control at the microscale was investigated by in situ compression testing in an electrolyte using a modified nanoindenter and a novel multiple load function. It was found that the potential dependent flow stress of NPG micropillars showed the same trend as corresponding results of NPG at the macroscale: significant increase at positive potential due to surface coverage of an OH- monolayer and reversible modulation with varying potentials. However, the elastic modulus is insensitive to the applied potential, which is in good agreement with corresponding results from in situ macro-compression experiments, but different to reported results of in situ dynamic mechanical analysis (DMA)

MM 61.3 Thu 16:15 IFW D

Impact of the precursor alloy composition on the mechanical properties of nanoporous gold — •Birthe Zandersons[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

Due to its chemical stability and the tunable structure size from a few to several hundred nanometers, nanoporous gold (NPG) is an attractive model system for small-scale material behavior. Its mechanical properties have been investigated over many years. Clear distinctions in stiffness and strength caused by variations of the solid fraction have been reported. Yet, a systematic investigation is still missing. Therefore, we systematically dealloyed AuAg alloys with Au amounts between 20 and 35 at.% electrochemically in 1 M $HClO_4$ or via free corrosion in concentrated HNO_3. Compression tests with continuous loading and with load/ unload protocols explored the stress-strain behavior and Young's modulus. We confirm a significant depending of the mechanical performance on the master alloy compositions and validate an impact of the topological genus.

MM 61.4 Thu 16:30 IFW D

In-depth porosimetry of pore evolution in low-k thin films — •Ahmed G. Attallah[1], Maciej Oskar Liedke[1], Nicole Koehler[2], Maik Butterling[1], Eric Hirschmann[1], Stefan E. Schulz[2], Ramona Ecke[2], and Andreas Wagner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, 01328 Dresden, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, 09126 Chemnitz, Germany

The development of the porous structure in low-k materials after conducting a thermal in-situ and ex-situ curing processes will be shown. Such a study has been performed by using positron annihilation spectroscopies (Lifetime and Doppler Broadening) and Fourier-transform infrared spectroscopy. The goal of this work is to take a closer look at the kinetics of the template removal which, in addition to the chemical structure of the matrix-template mixture, defines the created porosity. Positron lifetime shows that template decomposition starts at 473K and complete removal is accomplished at 723K. Additionally, it reveals template agglomeration and diffusion to the surface by creating channels that would affect the mechanical stability and the k-value. Definite curing temperature ranges for different processes (moisture removal, SiO_x network cross-linking, porogen decomposition) has been figured out by Doppler broadening spectroscopy during in-situ curing. Also, it shows a pore interconnectivity onset at 673K. Fourier-transform infrared spectroscopy results help for understanding the network changes during curing and confirmed positron results for template removal.

MM 61.5 Thu 16:45 IFW D

Scalable Structural Coloring Based on the Photonic Bandgap of Ordered Nanoporous Array — •Yudie Huang, Fanzhou Lv, Jiaxu Chen, Zhihang Wang, Shiyao Jia, Yi Wang, and Wenxin Wang — Harbin Engineering University , Harbin, China

Full structural coloring within the range of visible light has been fabricated through various methods due to the distinguished features of high saturation, durability and unfading. However, the reported prepared samples do not exhibit superior saturation compared to the natural structural color materials. Because of broad and multi-peaks surrounding profiles are existing in reflective ranges that obstruct the coloring saturation. Bandgap-assisted structural coloring based on sharp and less reflective peaks is highly recommended. Besides, color over a considerable spectral range remains stable. Here, we present a scalable and vivid structural coloring approach to acquire color with a more pure hue. (1) designing a metal-dielectric-metal structure system to narrow the reflect peaks. (2) regulating the parameters of the nanoporous array to reduce the number of reflectivity peaks and achieve bright and pure hue. The reflective peaks of nanoarray are adjusted and concentrated towards the position of photonic bandgap caused by highly ordered dielectric arrangement. (3) owing to the used fabrication method, the area of structural color presentation is sufficiently large to serve as commercial applications. Therefore, this scalable and vivid structural coloring proposal has promising application prospects in human daily life.

MM 61.6 Thu 17:00 IFW D

Atom Probe Tomography of Mesoporous Silica — •Kuan Meng, Patrick Stender, and Guido Schmitz — Stuttgart University, Germany

In order to visualize the porous structure of desiccant silica gel (orange) with atom probe tomography, the FIB cryogenic technique was used to prepare a solid tip sample by filling the pore with water vapor absorption and then freezing. In an attempt to understand the measurement result, this work was split into three parts of investigation in pure bulk silica as the pore wall material, pure water as the filler and the water-filled silica gel like a water-absorbed sponge respectively. In the first part, silica was thermally oxidized from silicon wafer and the tip samples were prepared with FIB Lift-Out technique. Its evaporation field was determined by measuring the Si/SiO2 interface in normal, vertical and reverse geometries. Moreover, the interface was found not flat. Secondly, water was measured by preparing an ice tip with the FIB cryogenic method. Despite the uncommon ring-like patterns in the detector view, the crystal ice peaks were found in the mass spectrum. Thirdly, a quasi-porous structure network was visualized in the case of the water-filled silica gel, revealing a promising future in the field of APT measurement for porous materials.

MM 62: Topical Session: Data Driven Materials Science - Machine Learning Applications (joint session MM/CPP)

Time: Thursday 17:30–19:00 Location: BAR 205

MM 62.1 Thu 17:30 BAR 205

How polymorphism of adsorbate molecules determines the physical properties of metal/organic interfaces: a large scale study — •Johannes J. Cartus, Andreas Jeindl, Lukas Hörmann, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria

The work function of metallic surfaces can be readily tuned via the interface dipole that emerges when adsorbing organic electron-donor or -acceptor molecules. Despite extensive research in the field and a wealth of experimental data available, it is presently still not possible to predict the magnitude of the dipole based on the choice of the interface materials alone. This is because molecular properties and the structure of adsorbate layers are rarely considered simultaneously, even though both are known to have great impact.

In this work, we present a systematic study of selected substrate/adsorbate combinations, for which we computationally determine the electronic structure of various surface polymorphs. This allows us to explore which kind of structures preferentially form for different molecule classes and directly relate them to the interface work function and other system properties.

MM 62.2 Thu 17:45 BAR 205

Investigation of short-range order in multicomponent alloys with the use of machine-learning interatomic potentials — •Tatiana Kostiuchenko[1], Alexander Shapeev[1], Fritz Körmann[2,3], and Andrey Ruban[4,5] — [1]Skolkovo Institute of Science and Technology, Moscow, Russia — [2]Delft University of Technology, Delft, The Netherlands — [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [4]KTH Royal Institute of Technology, Stockholm, Sweden — [5]Materials Center Leoben Forschung GmbH, Leoben, Austria

Multicomponent alloys, such as high-entropy alloys or multi-principal element alloys, are promising structural materials. However, the vast range of chemical compositions and long annealing times offer an opportunity for their study with ab initio methods. The drawback of ab initio methods is their huge computational costs. We address this drawback by developing efficient data-driven interaction models with accuracy close to those of ab initio methods, namely the low-rank interatomic potential (LRP) [Shapeev A., 2017]. They are used in a Canonical Monte Carlo algorithm as an “on-lattice” model that can take into account local lattice distortions. In this work, we investigate the equiatomic VCoNi system. It represents a medium-entropy alloy with a distorted fcc lattice which leads to an outstanding strength-ductility relationship as reported in [Sohn S. et al., 2019]. We simulate this system by including, implicitly, magnetism into LRP by fitting on spin-polarized DFT calculation. The LRP has the error of about 1-3 meV/atom and is used to study the formation of the short-range order.

MM 62.3 Thu 18:00 BAR 205

An equation for membrane permeability: Insight from compressed sensing — •Arghya Dutta and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Using a material’s structure and readily available properties to predict a difficult-to-measure but important property is crucial in natural sciences and engineering. Data mining—the process of discovering associations, correlations, and anomalies in data—can significantly facilitate the search for these generalized structure-property relationships by providing relevant descriptors. To give an example, the efficacy of a targeted drug depends on whether or not it can go through a cell membrane. This capacity is quantified by permeability which measures the drug’s flux across the membrane. However, calculating permeability is computationally expensive. In this presentation, I will discuss results from our ongoing search for a simple and interpretable equation, which is a function of key physical descriptors, for permeability using compressed sensing methods. This simplified description of permeability will allow simulation-free prediction, and, potentially, assist in rapid screening of candidate drug molecules.

MM 62.4 Thu 18:15 BAR 205

Transferable Gaussian Process Regression for prediction of molecular crystals harmonic free energy. — •Marcin Krynski[1] and Mariana Rossi[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

Organic molecular crystals are a large group of compounds with properties tied strongly to the crystallographic structure of their numerous polymorphs. While thermodynamic free energies are necessary for obtaining a reliable polymorph energy ranking[1,2], their inclusion in large-scale simulations for polymorph screening is challenging, because dispersion-corrected DFT accuracy is needed in order to capture the complex charge rearrangement and bond-softening. Therefore, to predict harmonic Helmholtz free energies, we devised a framework that employs the transferable Gaussian Process Regression model with Smooth Overlap of Atomic Positions[3] descriptors representing local atomic environments. We developed strategies based on farthest point sampling to minimize the size of the training set and to ensure statistical diversity. We benchmark our framework on a set of 444 hydrocarbon crystal polymorphs. Superior performance and high prediction accuracy, with mean absolute deviation below 0.1 meV/atom is achieved by a hyperparameter optimisation performed on empirical-potential models, ensuring sensitivity to longer-range structural patterns.

[1] J. Nyman and G. Day, *CrystEngComm* **17**, 5154 (2015);
[2] M. Rossi, P. Gasparotto, M. Ceriotti, *PRL* **117**, 115702 (2016);
[3] A. P. Bartók, R. Kondor, G. Csányi, *PRB* **87**, 184115 (2013).

MM 62.5 Thu 18:30 BAR 205

Bayesian modeling for potential energy surface minimization — •Estefania Garijo del Rio, Sami Juhani Kaapa, and Karsten Wedel Jacobsen — CAMD, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Computational simulations using electronic structure methods of materials and molecules require the (meta-)stable structure of the system under investigation to be known. In the absence of experimental structural data, the usual procedure is to use quantum chemistry codes together with some optimization algorithm to find successive approximations of a (local) minimum of the potential energy surface under the Born-Oppenheimer approximation. In this context, methods that incorporate machine learning surrogate models that are built on the fly to reduce the number of evaluations have recently gained popularity. Here, we explore and compare how different choices for the kernels can affect the performance of the optimization when Gaussian process regression is used to fit energies and forces.

MM 62.6 Thu 18:45 BAR 205

A computational route between band mapping and band structure — R. Patrick Xian[1], •Vincent Stimper[2], Marios Zacharias[1], Shuo Dong[1], Maciej Dendzik[1], Samuel Beaulieu[1], Matthias Scheffler[1], Bernhard Schölkopf[2], Martin Wolf[1], Laurenz Rettig[1], Christian Carbogno[1], Stefan Bauer[2], and Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

In solid state physics, the electronic band structure imprints the multidimensional relations between energy and momentum of periodically confined electrons. Photoemission spectroscopy has provided a reliable source of experimental validation for electronic structure theory and the understanding of electronic properties. Recent advancements in UV sources and detector technology leads to the growth of band mapping data in resolution, size and scale. This offers fresh opportunities for high-throughput material characterization. Here, we present an efficient probabilistic machine learning framework to connect photoemission band mapping with band structure calculations by reconstructing the full 3D valence band structure of tungsten diselenide within its first Brillouin zone. We then digitize the empirical shape of the reconstructed bands using orthonormal bases for multiscale sampling and comparison with theory. Our approaches open up avenues for the precise quantification of band structures and realize a viable path integrating band mapping data with computational materials science databases.

MM 63: Computational Materials Modelling - Electronic Structure of Complex Materials

Time: Thursday 17:30–19:00 Location: IFW A

MM 63.1 Thu 17:30 IFW A

Multistep stochastic mechanism polarization switching model — •Ruben Khachaturyan[1], Ankit Biswas[1], Anna Grünebohm[1], and Yuri Genenko[2] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum — [2]Institute of Materials Science, Technische Universität Darmstadt

The multistep stochastic mechanism (MSM) polarization switching model is a recent extension of the classical Kolmogorov-Avrami-Ishibashi model. It provides an easy way to describe polarization and strain kinetics of ferroelectrics with tetragonal symmetry. The model is now extended to rhombohedral and orthorhombic symmetries. The extended model can well fit experimental results, which evidence its capability to treat different symmetries. We try to utilize a machine learning algorithm based on linear regression to apply the modified MSM model to a system with a rhombohedral symmetry to get the best possible fitting of the experimental data. [1] **Stochastic multistep polarization switching in ferroelectrics**, Y.A. Genenko, R. Khachaturyan, J. Schultheiß, A. Ossipov, J. E. Daniels, and J. Koruza, **97(14)**, 144101 (2018)

MM 63.2 Thu 17:45 IFW A

First-principles investigation of the electromechanical response properties of ferroelectric HfO2 — •Sangita Dutta[1,2] and Jorge Iniguez[1,2] — [1]Luxembourg Institute of Science and Technology, Luxembourg — [2]University of Luxembourg, Luxembourg

Over the past few years, hafnia (HfO2) has been attracting attention due to its newly discovered ferroelectric behaviour [1]. This compound is a promising candidate for a variety applications ranging from ferroelectric memories to energy storage [2]. Interestingly, we note that, in spite of the very intense research focus on hafnia, a detailed understanding of response properties of ferroelectric hafnia is still missing in literature. In this present study, we compute the dielectric and piezoelectric responses of hafnia using first-principles density functional theory. More specifically, we work with the usual ferroelectric phase of hafnia (space group Pca21), and also investigate the variation of the electromechanical responses as a function of substitutional isovalent doping (i.e., Si, C, and other species replacing Hf atoms). In this talk, I will discuss our results and their implications for the optimization of the intrinsic response properties of ferroelectric hafnia.

Funded by the Luxembourg National Research Fund (PRIDE/15/10935404)

[1] T. S. Böscke, J. Muller, D. Bräuhaus, U. Schröder and U. Böttger.App. Phys. Lett. 99 (2011) [2] J. Muller, P. Polakowski, S. Muller and T. Mikolajick, ECS J.Solid State Sci.Technol. 4, N30-N35 (2015)

MM 63.3 Thu 18:00 IFW A

The Quantum Rectification Tensor of Three-Dimensional Materials — •Urmimala Dey[1,3], Oles Matsyshyn[1], Yan Sun[2], and Inti Sodemann[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden 01187, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — [3]Indian Institute of Technology Kharagpur, Kharagpur 721302, India

We report on the first realistic calculations of the Quantum Rectification Tensor (QRT) of three-dimensional materials without inversion symmetry for the Weyl semimetal TaAs and the ferroelectric insulator LiAsSe2. The QRT is a fundamental property of any material without inversion symmetry which is dictated entirely by its Berry phase geometry, and it is determined by the Quantum Rectification Sum Rule that contains the Berry Curvature Dipole but also additional interband optical shift current contributions. In three dimensions the QRT is dimensionless when measured in fundamental constants of nature, namely, in units of the quantum of conductance divided by the quantum of flux. We will discuss the importance of this QRT as a figure of merit in the search for technologically promising bulk photovoltaic materials.

MM 63.4 Thu 18:15 IFW A

computational screening for anderson insulators — •yazhi xu[1], xudong wang[2], riccardo mazzarello[1], and wei zhang[2] — [1]RWTH Aachen University, Aachen, Germany — [2]Xi'an Jiaotong University, Xi'an, China

Anderson insulators are characterized by charge localization induced by crystal disorder. Recently, it was shown that the compound Ge1Sb2Te4 can crystallize into a metastable rocksalt-like structure that exhibits an Anderson insulating phase stemming from vacancy disorder. Furthermore, an insulator-metal transition can be triggered in these compounds by thermal annealing, which leads to vacancy ordering. Here, we perform a systematic computational screening for Anderson insulators in IV1V2VI4 compounds based on density functional theory. We consider the rocksalt-like phase and carry out geometry optimization and bonding analysis to determine their stability. For the stable models, we determine the localization of the electronic states relevant to transport.

MM 63.5 Thu 18:30 IFW A

Addressing the conflict of locating solvated electrons in alkali metal doped zeolites — •Debalaya Sarker[1,2], Sergey V. Levchenko[1,2], and Matthias Scheffler[2] — [1]Skolkovo Institute of Science and Technology, Moscow, RU — [2]Fritz-Haber-Institut der MPG, Berlin, DE

Doping faujasite Y (FAU-Y), a nanoporous aluminosilicate zeolite, with alkali metal atoms M (Na, K, Cs, etc.) is a promising way to produce outstanding basic catalysts. The dopants, along with extraframework metal atoms, often form M_4^{+3} clusters inside zeolite pores: leaving the valence electron of the dopant solvated and available for catalysis. Despite extensive experimental efforts, the distribution of the dopants and solvated electrons remains debated till date [1,2]. Combining a cluster expansion model, parameterized with extensive PBE+vdW calculations, and *ab initio* atomistic thermodynamics, we address this issue. Further, the electronic structure is calculated with hybrid HSE06 functional for low-energy configurations. We find that at temperatures >850 K Na atoms in NaY zeolites with two extraframework atoms per unit cell on average redistribute so that areas with

lower and higher local concentrations emerge. The redistribution is driven by increased configurational disorder at both higher and lower concentrations. This explains why solvated electrons can be located inside both small and large cages in NaY, reconciling experiments assigning the solvated electrons to a particular pore type.
[1] A. R. Armstrong *et al.*, J. Am. Chem. Soc. **117**, 9087 (1995).
[2] W. Louisfrema *et al.*, Molecular Simulation **41**, 1371 (2015).

MM 63.6 Thu 18:45 IFW A

Comprehensive scan for nonmagnetic Weyl semimetals — •Qiunan Xu[1], Yang Zhang[1], Klaus Koepernik[2], Wujun Zhang[3], Jeroen van den Brink[2], Claudia Felser[1,4], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [3]School of Physical Science and Technology, ShanghaiTech University, Shanghai 200031, China — [4]Center for Nanoscale Systems,Faculty of Arts and Sciences, Harvard University,11 Oxford Street, LISE 308 Cambridge, MA 02138, USA

As the development of topological band theory, comprehensive databases about time reversal and crystalline symmetries protected nonmagnetic topological materials were developed via first-principles calculations recently. However, owing to the low symmetry requirement of Weyl points, the WSMs with Weyl points in arbitrary positions are still absent in the well-known databases. In this work, we develop an efficient algorithm to establish a database of nonmagnetic WSMs with Weyl points near Fermi level based on the total experimental noncentrosymmetric crystal structures in ICSD. Totally 49 Weyl semimetals were discovered to have nearly clean Fermi surface and Weyl points near Fermi level within 300 meV, and 12 of them are chiral structures hosting the quantized circular photogalvanic effect. In addition, the nonlinear optical response is studied and giant shift current is explored in the end. Besides nonmagnetic WSMs, our powerful tools can also be used in the discovery of magnetic topological materials.

MM 64: Mechanical Properties: Plasticity, fracture, fatigue, wear - II

Time: Thursday 17:30–19:00 Location: IFW B

MM 64.1 Thu 17:30 IFW B

Can machine learning be used to extract single phase properties based on nanoindentation mapping? A case study in steels — •Robin Jentner[1], Kinshuk Srivastava[2], Bastian Philippi[2], Christoph Kirchlechner[1], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]AG der Dillinger Hüttenwerke, 66763 Dillingen, Germany

Advanced high strength steels exhibit an intricate microstructure comprising of several different phases and interfaces that determines the mechanical behavior of the bulk material. In order to examine the mechanical behavior of each individual phase, micro pillar compression tests have been used. However, micro pillar compression is tedious and time consuming. In this work, we explore the capability of high throughput nanoindentation combined with k-means clustering to determine the mechanical properties of each single phase.

We have trained first the k-means clustering method with a two-phase laboratory sample which was finally applied to a HSLA bainitic steel consisting of three different phases. The clustering revealed two to three clusters in the first case and at least five clusters for the bainitic steel. To unravel the origin of the additional clusters we have performed correlative microscopy and found that indents close to grain or phase boundaries are responsible for them. Based on the obtained results we conclude that analyzing the mechanical properties of complex bulk materials by k-means clustering provide a suitable microstructural characterization method, which will be discussed in the talk.

MM 64.2 Thu 17:45 IFW B

Atomistic and continuum simulation of brittle and ductile crack in titanium aluminide single and bi-crystals — •Anupam Neogi, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-Universität Bochum, Germany

Ti-Al alloys are well known for their excellent mechanical properties. However, they often exhibit low-ductility, which leads to in-service brittle failure. The fracture behavior of metallic materials is primarily governed by the competition between emission of dislocations and Griffith cleavage at the crack tip. In two-phase Ti-Al however, this simple picture is questionable. Here the anisotropy of the major phases, γ-TiAl and α_2-Ti$_3$Al, with a limited number of slip systems, leads to complex crack propagation mechanisms.

We investigate crack propagation under mode I loading in single-crystal γ and α_2 Ti-Al, as well as at γ/γ interfaces, using anisotropic linear elastic fracture mechanics (LEFM) and atomistic simulations. The latter show a significant directional dependence of crack tip behavior. For instance, a (111)-crack in γ-TiAl propagates by Griffith cleavage along $[\bar{2}11]$, but by dislocation emission along $[11\bar{2}]$. Basal cracks in α_2-Ti$_3$Al are generally assumed to propagate in a brittle manner, but we observe nucleation of dislocations if the crack propagates along $[10\bar{1}0]$. The complexity increases in the vicinity of γ/γ interfaces, in which the mechanism depends on the orientation of the crack plane with respect to the interface. Nevertheless, it is the remarkable conclusion of this study that the predictions of LEFM agree well - qualitatively and quantitatively - with atomistic simulations.

MM 64.3 Thu 18:00 IFW B

Multiscale quantum classical modelling of the interaction of crack systems with defects in diamond — •James Brixey and James Kermode — University of Warwick, Coventry, United Kingdom

Diamond is a material with many applications in industry and science, in particular for cutting and drilling. However, its brittle nature leads to catastrophic failure by fracture, and in order to reduce the probability of failure, it is important to understand as much about the atomic-scale details fracture as possible. Building on earlier work that found that individual boron impurities can form microscopic ridges in silicon, at certain crack speeds [Kermode et al, Nat. Comm (2013)], it is reasonable to postulate that single substitutional nitrogen in diamond might have interesting effects of a similar nature. In order to understand fracture of brittle materials, careful modelling of both the long-range stress field and the short-range bond breaking is required. To capture this, a multiscale (QMMM) model has been developed, using Density Functional Theory to accurately capture the activity far from equilibrium near the crack tip, whilst simultaneously capturing the elastic field interaction using an empirical interatomic potential. Preliminary results of our model will be presented, both for pure and defect containing diamond.

MM 64.4 Thu 18:15 IFW B

***In silico* experiments on mechanics of TiN/AlN superlattices: an MD study** — •Lukas Löfler[1], Matthias Bartosik[2], Paul Heinz Mayrhofer[2], and David Holec[1] — [1]Montanuniversität Leoben — [2]TU Wien

Nitride-based thin films are commonly used to protect components from harsh environments and high loading occurring in modern applications. A way to improve the mechanical properties of such coatings is to carefully design the microstructure. For instance, combining two materials in a coherent multilayer arrangement with layer thicknesses in the nm range (termed *superlattice*) can enhance both hardness and fracture toughness; two material properties that often seem to be mutually exclusive.

Utilizing molecular dynamics (MD), indentation and tensile loading simulations were performed to investigate the mechanical response of AlN/TiN superlattices on different loading scenarios. For the indentation, a spherical object was gradually moved into the coating displacing atoms. For the tensile loading, the atoms at the top and bottom of the coating were moved so to apply axial tension. For both setups, the forces, stresses and the nucleation of dislocations were analyzed. To gain more insight into the nucleation process of the dislocations, different cores and their structures were calculated for the most common slip systems.

MM 64.5 Thu 18:30 IFW B

Effect of lattice misift on the deformation behaviour of two-phase lamellar TiAl alloys — •Ashish Chauniyal and Rebecca

Janisch — ICAMS, Ruhr Universit
"at Bochum

Deformability and strength of two phase TiAl alloys strongly depends on the presence of different interfaces in their microstrucure. Two phase TiAl alloys consists of face centered tetragonal γ(TiAl) phase and hexagonal $\alpha_2(Ti_3Al)$ phase. The interfaces in lamellar alloys are either γ/γ or α_2/γ. Lattice misfits arise due to different crystal structures at α_2/γ interface or due to tetragonality at γ/γ interfaces. A coherent interface, with matching lattice points, leads to coherency stresses in lamellae, whereas a semi-coherent interface has misfit dislocations. Using molecular dynamics simulations we study the deformation behaviour of coherent and semi-coherent interfaces by carrying uniaxial tensile tests on bi-layer specimens of α_2,γ. We quantify the relation between volume fraction and coherency stresses in lamellae and distinguish the role of volume fraction and individual lamellar size on deformation behaviour. Coherency stresses in lamellae lead to early yielding of α_2,γ bilayers which could be the origins of the observed microplasticity in TiAl alloys. Furthermore, we show that misfit dislocations at the interfaces create local stress fluctuations within the lamellae, which in turn, lead to dislocation nucleation. Thus, we distinguish different dislocation nucleation mechanisms in coherent and semi-coherent interfaces in correlation with changing stress states caused due to lattice misfit.

MM 64.6 Thu 18:45 IFW B

Mechanical property gradients of spider attachment hairs — •Silja Flenner[1], Clemens Schaber[2], Imke Greving[1], Igor Krasnov[1], Manfred Burghammer[3], Martin Rosenthal[3], Stanislav Gorb[2], and Martin Müller[1] — [1]Helmholtz-Zentrum Geesthacht, Germany — [2]Institute of Zoology, Kiel University, Germany — [3]ESRF, Grenoble, France

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

The technique of high spatial resolution mapping based on scanning X-ray nanobeam diffraction and small-angle scattering was used to study the hairy attachment system of spiders. Each point of a map represents a structural parameter such as orientation or scattered intensity extracted from a diffraction pattern. Additional nanotomography measurements allows to correlate the structural parameters with 3D data. These techniques were combined with an in situ attachment/detachment procedure. The goal of our study is to gain an in-depth understanding of the structures and mechanical properties of single hairs during the attachment and detachment process to a surface.

MM 65: Nanomaterials - II

Time: Thursday 17:30–19:00 Location: IFW D

MM 65.1 Thu 17:30 IFW D

3D X-ray Diffraction Microscopy (3DXRD) using high resolution X-ray nanodiffraction — •Hergen Stieglitz[1], Johan Hektor[2], Anton Davydok[1], Christina Krywka[1], and Martin Müller[1] — [1]Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]DESY, Hamburg, Germany

The existing technology called 3DXRD is a well-established technique to map the grain structure of polycrystalline systems (e.g. metals). This technology is based on reconstruction algorithms which trace the positions of multiple Bragg-Peaks as a function of the rotation angle during sample rotation. These algorithms rely on that the diffraction spots do not overlap. Therefore there is a limit on the maximum number of grains, or equivalently, the smallest grain size that can be mapped.

The newly implemented nano grain mapping experiment at the beamline P03 (PETRA III) is based on scanning 3DXRD and utilizes a nano-focused X-ray synchrotron beam to examine very fine-grained systems. With respect to the small beam size of about 250 nm cross section, the precise positioning of the sample becomes more important to secure a constant gauge volume. Otherwise some grains may be outside the gauge volume in some scans, therefore they cannot be traced and produce mistakes while reconstructing.

To meet this challenge a stable and wobble-free rotation stage is in operation to ensure a constant gauge volume. A laser interferometer based feedback loop compensates the runout of the sample during rotation. Results of the very first experiments will be shown.

MM 65.2 Thu 17:45 IFW D

Epitaxial NbP and TaP Weyl Semimetal thin films - a new playground for topological heterostructures — •Amilcar Bedoya Pinto, Avanindra Kumar Pandeya, Defa Liu, Hakan Deniz, Kai Chang, Hengxin Tan, Hyeon Han, Jagannath Jena, Ilya Kostanovskiy, and Stuart Parkin — Max Planck-Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Weyl Semimetals (WSMs), a recently discovered topological state of matter, exhibit an electronic structure governed by linear band dispersions and degeneracy (Weyl) points leading to rich physical phenomena, which are yet to be exploited in thin film devices. While WSMs were established in the monopnictide compound family several years ago, the growth of thin films has remained a challenge. Here, we report the growth of epitaxial thin films of NbP and TaP by means of molecular beam epitaxy. Single crystalline films are grown on MgO (001) substrates using thin Nb (Ta) buffer layers, and are found to be tensile strained (1%) and with slightly P-rich stoichiometry with respect to the bulk crystals. The resulting electronic structure exhibits topological surface states characteristic of a P-terminated surface and linear dispersion bands featuring a Fermi-level shift of -0.2 eV with respect to the Weyl points. The growth of epitaxial thin films allows the use of strain and controlled doping to tune the electronic structure of Weyl Semimetals on demand, paving the way for the rational design and fabrication of electronic devices ruled by topology.

MM 65.3 Thu 18:00 IFW D

Defect and interlayer engineering in transition metal dichalcogenides for enhancing potassium storage — •Yuhan Wu, Chenglin Zhang, and Yong Lei — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693, Ilmenau, Germany

The role of the defect and interlayer engineering in two-dimensional transition metal dichalcogenides is explored for potassium storage. Molybdenum disulfide was selected as an example; the expanded interlayer spacing and defects in the basal planes are used as the anode of potassium-ion battery with voltage window of 0.5*2.5 V, which ensure the intercalation reaction rather than a conversion reaction takes place to store K-ions in the van der Waals gaps. In comparison to the defect-free counterpart with pristine interlayer spacing, the MoS2 nanoflowers showed enhanced potassium storage performance. Kinetic analysis verifies that the K-ion diffusion coefficient and surface charge storage are both enhanced. The collective effects of expanded interlayer spacing and additionally exposed edges induced by the in-plane defects enable facile potassium ion intercalation, rapid potassium ion transport and promoted surface K-ion adsorption at the same time.

MM 65.4 Thu 18:15 IFW D

Atom Probe Tomography of self-assembled Monolayers — •Helena Solodenko and Guido Schmitz — Institute for Material Science, Heisenbergstr. 3, 70569 Stuttgart

In order to achieve molecular heterogeneous catalysis in confined geometries, catalyst molecules are linked to nanometer-sized pores within a matrix. The linkage of catalyst to the pores is crucial and therefore this project focuses on this aspect. We utilize simple model molecules which form by self-organization, so-called self-assembled monolayers (SAM), and investigate them by atom probe tomography (APT). This technique excels at chemical sensitivity and provides furthermore three-dimensional spatial information of the probed samples. The goal is to achieve physical understanding of field desorption of organic molecules under high electric fields. Experiments are conducted by preparation of nanometer-sized metallic needles, which are cleaned by field-evaporation and then coated by dipping in the according solution of thiol-based SAMs for several hours. The resulting monolayer has a thickness of less than two nanometers and is analyzed by laser-assisted APT. The carbon chains break under the influence of the high electric fields and corresponding molecular fragments are detected by time-of-flight mass spectrometry. The reconstruction reveals an ordered evaporation sequence of the molecule chain down to the substrate and provides information of surface coverages of the SAMs. Furthermore, SAMs of phosphonic acids are used, which bind to oxide materials like SiO2, Al2O3 and their evaporation behavior is compared to thiol-based SAMs.

MM 65.5 Thu 18:30 IFW D

A plasmonic absorber based on the multi-order square array of gold nanocylinders — •Zhi-Hang Wang[1], Yudie Huang[1], Peng Xie[2], Jiaxu Chen[1], Fanzhou Lv[1], Shiyao Jia[1], Yi Wang[1], Wei Wang[2], and Wenxin Wang[1] — [1]Photonic Materials Group, College of Physics and Optoelectronic Engineering, Harbin Engineering University, Harbin, China — [2]College of Physical Science and Technology, Sichuan University, Chengdu, China

Plasmonic structures are known to have strong confinement for incident light at the nanoscale. Here, a plasmonic absorber based on a sandwich nanostructure consisting of multi-order square array of 'gold cylinders- dielectric space-gold resisting layer' is studied. Thanks to the numerical simulation by FDTD, longitudinal modes at the lateral surface of gold nanocylinders and the hybrid plasmon modes at the interfaces between gold and the dielectric space are demonstrated. Furthermore, simultaneously existing of the longitudinal modes and the hybrid plasmon modes arise the plasmon-plasmon coupling at 0.9 μm and 1.4 μm. These distinctive plasmon-plasmon coupling modes result in the anti-cross splitting phenomena in the dispersion diagrams. Finally, the simulated numerical performance is designed to be verified by the experimental measurements. This work demonstrates the sandwich structure based on multi-order square array of nanocylinders-dielectric space-gold resisting layer has good potential in the field of manipulating light at nanoscale with a low-cost, large-area sample fabrication process, which opens up many promising applications such as optical absorption and strong plasmon-plasmon interaction.

MM 65.6 Thu 18:45 IFW D

The Special Role of Oxygen in the Growth of Oxide-based Compound Nanowires: Experiments and Simulation — •Jasmin-Clara Bürger, Sebastian Gutsch, and Margit Zacharias — Department of Microsystems Engineering - IMTEK, Laboratory for Nanotechnology, University of Freiburg, Georges-Köhler-Allee 103, 79110 Freiburg, Germany

The growth of oxide-based compound nanowires allows for a huge field of applications due to their unique properties. However, systematic studies on the growth of SnO2 nanowires and the influences of the individual growth parameters on the resulting structures are rare. Especially for the usage in applications, a controlled and reliable growth process and the understanding of its manipulation are becoming necessary for a purposive resulting morphology. Particularly, the VLS growth and allied methods supported by a carbothermal reduction in a horizontal tube furnace are possessing a high sensitivity to a large quantity of influencing parameters. Recently, we reported on the inhibition of the NW growth provoked by a high oxygen concentration and the timing of the oxygen inflow due to the formation of an oxidic shell.[1] Neither oxygen nor SnO2 are soluble in the Au catalyst particle. Nevertheless, we showed that the oxygen inflow is necessary to grow these NWs.[1] Therefore, a control of the Sn/O ratio at the sample sites becomes mandatory.[1] We support our experiments with numerical simulations.

[1] J.-C. Bürger et al., J. Phys. Chem. C 122 (2018) 24407-24414