

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

Astrid Pundt
Institut für Angewandte Materialien-Werkstoffkunde (IAM-WK)
Karlsruher Institut für Technologie (KIT)
Kaiserstraße 12
76131 Karlsruhe
astrid.pundt@kit.edu

Overview of Invited Talks and Sessions

(Lecture halls H44, H45, and H46; Poster P2)

Invited Talks

MM 1.1	Mon	9:30–10:00	H44	A novel mechanism to generate metallic single crystals — ●CAROLIN KÖRNER, JULIAN PISTOR, JOHANNES BÄREIS, MATTHIAS MARKL
MM 11.1	Tue	9:30–10:00	H44	Fast calorimetry: studying phase transitions in slow motion — ●JÖRG F. LÖFFLER
MM 19.1	Wed	9:30–10:00	H44	High-Entropy Alloys: Materials design in high dimensional chemical space from ab initio thermodynamics — ●FRITZ KÖRMANN
MM 27.1	Thu	9:30–10:00	H44	Crystal rotation kinematics during the tribological loading of high-purity copper — ●CHRISTIAN GREINER

Invited Talks of the joint Symposium SKM Dissertation Prize 2022 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:15–10:45	H2	Charge localisation in halide perovskites from bulk to nano for efficient optoelectronic applications — ●SASCHA FELDMANN
SYSD 1.2	Mon	10:45–11:15	H2	Nonequilibrium Transport and Dynamics in Conventional and Topological Superconducting Junctions — ●RAFFAEL L. KLEES
SYSD 1.3	Mon	11:15–11:45	H2	Probing magnetostatic and magnetotransport properties of the antiferromagnetic iron oxide hematite — ●ANDREW ROSS
SYSD 1.4	Mon	11:45–12:15	H2	Quantum dot optomechanics with surface acoustic waves — ●MATTHIAS WEISS

Invited Talks of the joint Symposium From Physics and Big Data to the Design of Novel Materials (SYNM)

See SYNM for the full program of the symposium.

SYNM 1.1	Mon	15:00–15:30	H1	How to tackle the "I" in FAIR? — ●CLAUDIA DRAXL
SYNM 1.2	Mon	15:30–16:00	H1	Beyond the average error: machine learning for the discovery of novel materials — ●MARIO BOLEY, SIMON TESHUVA, FELIX LUONG, LUCAS FOPPA, MATTHIAS SCHEFFLER
SYNM 1.3	Mon	16:00–16:30	H1	The Phase Diagram of All Inorganic Materials — ●CHRIS WOLVERTON
SYNM 1.4	Mon	16:45–17:15	H1	Automated data-driven upscaling of transport properties in materials — ●DANNY PEREZ, THOMAS SWINBURNE
SYNM 1.5	Mon	17:15–17:45	H1	Data-driven understanding of concentrated electrolytes — ●ALPHA LEE

Invited Talks of the joint Symposium United Kingdom as Guest of Honor (SYUK)

See SYUK for the full program of the symposium.

SYUK 1.1	Wed	9:30–10:00	H2	Structure and Dynamics of Interfacial Water — ●ANGELOS MICHAELIDES
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SYUK 1.2	Wed	10:00–10:30	H2	A molecular view of the water interface — ●MISCHA BONN
SYUK 1.3	Wed	10:30–11:00	H2	Motile cilia waves: creating and responding to flow — ●PIETRO CICUTA
SYUK 1.4	Wed	11:00–11:30	H2	Cilia and flagella: Building blocks of life and a physicist’s playground — ●OLIVER BÄUMCHEN
SYUK 1.5	Wed	11:45–12:15	H2	Computational modelling of the physics of rare earth - transition metal permanent magnets from SmCo₅ to Nd₂Fe₁₄B — ●JULIE STAUNTON
SYUK 2.1	Wed	15:00–15:30	H2	Hysteresis Design of Magnetic Materials for Efficient Energy Conversion — ●OLIVER GUTFLEISCH
SYUK 2.2	Wed	15:30–16:00	H2	Non-equilibrium dynamics of many-body quantum systems versus quantum technologies — ●IRENE D’AMICO
SYUK 2.3	Wed	16:00–16:30	H2	Quantum computing with trapped ions — ●FERDINAND SCHMIDT-KALER
SYUK 2.4	Wed	16:45–17:15	H2	Breaking the millikelvin barrier in cooling nanoelectronic devices — ●RICHARD HALEY
SYUK 2.5	Wed	17:15–17:45	H2	Superconducting Quantum Interference Devices for applications at mK temperatures — ●SEBASTIAN KEMPF

Invited Talks of the joint Symposium Frontiers of Electronic-Structure Theory: Focus on Artificial Intelligence Applied to Real Materials (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Thu	15:00–15:30	H1	Machine-learning-driven advances in modelling inorganic materials — ●VOLKER L. DERINGER
SYES 1.2	Thu	15:30–16:00	H1	Machine-Learning Discovery of Descriptors for Square-Net Topological Semimetals — ●EUN-AH KIM
SYES 1.3	Thu	16:00–16:30	H1	Four Generations of Neural Network Potentials — ●JÖRG BEHLER
SYES 1.4	Thu	16:30–17:00	H1	Using machine learning to find density functionals — ●KIERON BURKE
SYES 1.5	Thu	17:00–17:30	H1	Coarse graining for classical and quantum systems — ●CECILIA CLEMENTI

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H44	Invited Talk Carolin Körner
MM 2.1–2.10	Mon	10:15–13:00	H44	Computational Materials Modelling: Energy Materials
MM 3.1–3.9	Mon	10:15–12:45	H45	Microstructures and Phase Transformations: Metals & Alloys
MM 4.1–4.10	Mon	10:15–13:00	H46	Structural Materials
MM 5.1–5.1	Mon	15:00–15:30	H44	Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 1
MM 6.1–6.10	Mon	15:45–18:30	H44	Computational Materials Modelling: Defects / Alloys
MM 7.1–7.5	Mon	15:45–17:00	H45	Microstructures and Phase Transformations: Oxides & Perovskites
MM 8.1–8.10	Mon	15:45–18:30	H46	Materials for Storage and Conversion of Energy
MM 9.1–9.4	Mon	17:15–18:30	H45	Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 2
MM 10.1–10.30	Mon	18:00–20:00	P2	Poster Session 1
MM 11.1–11.1	Tue	9:30–10:00	H44	Invited Talk Jörg F. Löffler
MM 12.1–12.10	Tue	10:15–13:00	H44	Computational Materials Modelling: Physics of Ensembles 1
MM 13.1–13.7	Tue	10:15–13:00	H45	Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 3
MM 14.1–14.5	Tue	10:15–11:30	H46	Materials for Storage and Conversion of Energy (joint session MM/KFM)
MM 15.1–15.5	Tue	11:45–13:00	H46	Hydrogen in Materials: Hydrogen Effects
MM 16.1–16.4	Tue	14:00–15:00	H44	Mechanical Properties
MM 17.1–17.5	Tue	14:00–15:15	H46	Hydrogen in Materials: Hydrogen Storage
MM 18.1–18.43	Tue	17:30–20:00	P2	Poster Session 2
MM 19.1–19.1	Wed	9:30–10:00	H44	Invited Talk Fritz Körmann
MM 20.1–20.10	Wed	10:15–13:00	H44	Computational Materials Modelling: HEA, Alloys & Nanostructures
MM 21.1–21.10	Wed	10:15–13:00	H45	Transport in Materials: Thermal transport
MM 22.1–22.8	Wed	10:15–13:00	H46	Data Driven Materials Science: Experimental Data Treatment and Machine Learning

MM 23.1–23.10	Wed	15:45–18:30	H44	Computational Materials Modelling: Magnetic & Electrical Properties
MM 24.1–24.7	Wed	15:45–18:30	H45	Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 4
MM 25.1–25.8	Wed	15:45–18:30	H46	Data Driven Materials Science: Computational Frameworks / Chemical Complexity
MM 26	Wed	18:45–20:15	H44	Members’ Assembly
MM 27.1–27.1	Thu	9:30–10:00	H44	Invited Talk Christian Greiner
MM 28.1–28.5	Thu	10:15–11:30	H44	Transport in Materials: Diffusion / Electrical Transport & Magnetism
MM 29.1–29.5	Thu	10:15–11:30	H45	Data Driven Materials Science: Design of Functional Materials
MM 30.1–30.10	Thu	10:15–13:00	H46	Liquid and Amorphous Metals
MM 31.1–31.5	Thu	11:45–13:00	H44	Computational Materials Modelling: Physics of Ensembles 2
MM 32.1–32.5	Thu	11:45–13:00	H45	Nanomaterials: Surface Effects
MM 33.1–33.10	Thu	15:45–18:30	H44	Computational Materials Modelling: Process Schemes / Oxides
MM 34.1–34.10	Thu	15:45–18:30	H45	Data Driven Materials Science: Interatomic Potentials / Reduced Dimensions
MM 35.1–35.10	Thu	15:45–18:30	H46	Nanomaterials: Structure & Properties

Members’ Assembly of the Metal and Material Physics Division

Wednesday 18:45–20:15 H44

MM 1: Invited Talk Carolin Körner

Time: Monday 9:30–10:00

Location: H44

Invited Talk

MM 1.1 Mon 9:30 H44

A novel mechanism to generate metallic single crystals — ●CAROLIN KÖRNER, JULIAN PISTOR, JOHANNES BÄREIS, and MATTHIAS MARKL — Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

Single crystals are used for high strength materials with high creep resistance such as turbine blades from nickel-base superalloys. The fabrication techniques applied to produce single crystals involve highly controlled and therefore relatively slow crystallization. For turbine blades, the Bridgman technique, i.e. investment casting combined with directional 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 (AM) in the powder bed. These AM single crystals develop under rapid and directional solidification conditions with solidification microstructures one or two orders of magnitude finer than in the conventional Bridgman process. In addition, the underlying mechanism to generate the single crystal is based on thermo-mechanical provoked texture formation. The latter allows a very precise orientation of the single crystal. A manipulation of the orientation is possible by applying adequate process strategies. The basis mechanisms leading to the single crystal and the implications on the resulting properties are discussed.

MM 2: Computational Materials Modelling: Energy Materials

Time: Monday 10:15–13:00

Location: H44

MM 2.1 Mon 10:15 H44

Importance of electronic correlations in exploring the exotic phase diagram of Li ion battery cathodes — ●HRISHIT BANERJEE^{1,2}, CLARE P. GREY¹, and ANDREW J. MORRIS² — ¹Department of Chemistry, University of Cambridge, UK — ²School of Metallurgy and Materials, University of Birmingham, UK.

We explore electronic and magnetic states of layered Li_xMnO_2 , a well known cathode material for Li ion batteries, as a function of states of charge x , using *ab-initio* dynamical mean-field theory. Projecting onto low-energy subspace of Mn $3d$ states, and solving a multi-impurity problem, we find that an antiferromagnetic insulating state appears in LiMnO_2 , with a moderate Néel temperature in agreement with experimental studies. As the system is delithiated we find various exotic states emerge such as ferrimagnetic correlated metals, charge ordered ferromagnetic correlated metals with large quasiparticle weight, ferromagnetic metals with small quasiparticle weight, as a function of various states of delithiation of LiMnO_2 and finally an antiferromagnetic insulator for the fully delithiated state, which is albeit unstable. At moderate states of charge, $x=0.67$ - 0.33 , a mix of $+3/+4$ formal oxidation states of Mn is observed, while its overall nominal oxidation state changes from $+3$ in LiMnO_2 to $+4$ in MnO_2 . In all these cases the high-spin state emerges as the most likely state. The quasiparticle peaks in the correlated metallic states could be attributed to polaronic states. We explore the temperature vs. state of charge phase diagram and conclude that the state of charge is a key ingredient for the emergence of the exotic correlated phase transitions in this material.

MM 2.2 Mon 10:30 H44

Quantum-mechanical characterization of sulfur/carbon copolymer cathodes for Li-S batteries — ●POUYA PARTOVI-AZAR — MLU Halle-Wittenberg, Germany

Lithium-sulfur (Li-S) batteries are among the candidates for next-generation energy-storage systems thanks to their high energy density which arises from a high lithium capacity of elemental sulfur. However, cycling performance of Li-S batteries is drastically declined by a reversible capacity fade which is brought about by the diffusion of soluble Li-polysulfides through the electrolyte.^[1,2]

It has been recently shown that polymeric sulfur cathodes exhibit a promising performance in limiting the shuttle effect during the discharge.^[2] However, a clear atomistic picture on the favorable structures and their lithiation mechanism is still not fully established.

Here, we report our recent works on structural and electronic properties as well as finite-temperature vibrational spectra of polymeric sulfur cathodes, namely sulfur/1,3-diisopropenylbenzene^[3] and sulfur/polyacrylonitrile-based nanofiber^[4] co-polymers obtained through quantum-mechanical calculations.

[1] Qing Zhang *et al.*, *Adv. Sci.* 2103798 (2021); [2] G. Bieker *et al.*, *Commun. Mater.* 2, 37 (2021); [3] R. Kiani *et al.*, *ChemPhysChem*, doi: 10.1002/cphc.202100519; [4] P. Partovi-Azar *et al.*, *Phys. Rev. Applied* 1, 014012 (2018); P. Partovi-Azar, *under review* (2022)

MM 2.3 Mon 10:45 H44

Si nanostructure formation in quenched AlSi μ -droplets for application as anode material in lithium-ion-batteries — ●DAVID TUCHOLSKI and KARL-HEINZ HEINIG — Helmholtz-Center Dresden-Rossendorf, Dresden, Germany

We report on 3D lattice kinetic Monte Carlo (3DkMC) simulation of nanostructure formation during rapid quenching in gas-atomization (up to 10^8K/s) of droplets of AlSi alloy melt. The nanostructured Si particles (with the Al selectively etched away) promise to enable about 10x the capacity of the current state-of-the-art graphite in lithium-ion batteries by mitigating Si pulverization.

This work reproduces the experimentally found nanosponge and core-shell particles and reveals heteronucleation at Al_2O_3 sites resulting from trace oxygen at the surface as the formation mechanism for core-shell particles.

The computer simulation uses a memory-efficient bit-encoded lattice, enabling large scale atomistic calculations, while kinetics is implemented via CPU-efficient bit-manipulation for atom jumps between lattice sites. The jump probabilities are described by the metropolis algorithm with a look-up-table of energies calculated with an angular dependent potential for the Si-Al-Au system in LAMMPS.

This work is supported by the federal ministry for economic affairs and climate protection under grant number 01221755/1.

MM 2.4 Mon 11:00 H44

Tackling structural complexity in $\text{Li}_2\text{S-P}_2\text{S}_5$ solid-state electrolytes using Machine Learning — ●TABEA HUSS, CARSTEN STAACKE, JOHANNES MARGRAF, KARSTEN REUTER, and CHRISTOPH SCHEURER — Fritz-Haber-Institut der MPG

The lithium thiophosphate (LPS) material class provides promising candidates for solid-state electrolytes (SSE) in lithium ion batteries due to high lithium ion conductivities, non-critical elements, and low material cost. LPS materials are characterized by complex thiophosphate microchemistry and structural disorder influencing the material performance. *Ab-initio* studies probing lithium ion conductivity are constrained in system size and simulated time scales. This limits the transferability of computational results to industrial applicable LPS materials. Therefore, we present the development of a data efficient training protocol for the LPS material class using the Gaussian Approximation Potential (GAP). The GAP model can likewise describe crystal and glassy materials and different P-S connectivities P_mS_n . We apply the GAP model to probe lithium ion conductivity and discuss the influence of poly-anions on the latter. The sampling approach allows for a variety of extension and transferability to other SSE.

MM 2.5 Mon 11:15 H44

Exploration of cathode-stable layered solid-state electrolytes — ●SINA ZIEGLER, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz-Haber-Institut der MPG, Berlin, Germany

Promising higher safety and capacity, all-solid-state lithium batteries are envisioned to replace standard lithium-ion batteries in the future. Lithium thiophosphates achieve the highest Li ion conductivities

of SSEs to date exceeding liquid electrolytes at 10 mS/cm [1].

Until now, the instability of most SSEs towards high-performance electrodes remains a critical challenge, with hardly any known SSE withstanding the reducing/oxidizing conditions at the lithium metal anode and/or high-voltage cathodes or forming electrochemically benign interfaces with the electrode active materials.

To address this issue, we investigate the concept of rare earth lithium halides as a material-efficient, nm thick cathode coating in contact with thiophosphate electrolytes as they provide wide electrochemical stability windows (0.36-6.71 V vs Li/Li⁺) as well as good chemical and thermodynamic stability [2,3].

In order to validate this approach, the thermodynamic stabilities of the emerging SSE / halide interfaces are examined by ab initio thermodynamics to screen reaction free enthalpies of possible interface reactions. Furthermore, (stable) products of selected material combinations are surveyed for sufficient lithium ion mobility.

[1] C. Wang et al., Energy Environ. Sci., 2021, 14, 2577 [2] J. Liang et al., Acc. Chem. Res. 2021, 54, 1023-1033 [3] K. Kim et al., Chem. Mater. 2021, 33, 10, 3669-3677

15 min. break

MM 2.6 Mon 11:45 H44

Ab-initio core spectroscopy of LiCoO₂ and CoO₂ — DANIEL DUARTE RUIZ and ●CATERINA COCCHI — Carl von Ossietzky Universität Oldenburg, Institut für Physik, Oldenburg, Deutschland

X-ray absorption spectroscopy (XAS) is one of the most widely used technique to study the electronic structure of cathode active materials in operando conditions. From a theoretical point of view, many-body perturbation theory on top of density-functional theory [1] is the state of the art in the prediction of XAS and in the interpretation of corresponding experimental results. In this work, we investigate core spectroscopy in LiCoO₂ and CoO₂, considering excitations from the Co K- and L23-edges as well as from the O K-edge. Our results, in agreement with experimental data, indicate that excitonic effects are negligible for the absorption spectra. The spectral fingerprints are well reproduced already by the independent particle approximation and, on a qualitative level, by the atomic, orbital features in the projected density states. These findings suggest that monitoring the electronic structure of LiCoO₂ during the delithiation process is sufficient to capture the evolution of XAS signatures even in a possible high-throughput fashion.

[1] C. Vorwerk et al. Electron. Struct. 1, 037001 (2019)

MM 2.7 Mon 12:00 H44

High-throughput computational screening of fast Li-ion conductors — ●TUSHAR THAKUR, LORIS ERCOLE, and NICOLA MARZARI — THEOS, EPFL, Switzerland

We present a high-throughput computational screening to find fast Li-ion conductors to identify promising candidate materials for application in solid-state electrolytes. Starting with ~30,000 experimental structures sourced from COD, ICSD and MPDS repositories, we performed highly automated calculations using AiiDA at the level of Density Functional Theory (DFT) to identify electronic insulators and to estimate lithium ion diffusivity using the pinball model [1] which describes the potential energy landscape of diffusing lithium at near DFT level accuracy while being orders of magnitude faster. We present the workflow where the accuracy of the pinball model is improved self-consistently and which is necessary in automatically running the thousands of required calculations and analysing their results. Promising conductors are further studied with first principles Molecular Dynamics simulations.

[1] Kahle, L. et al Modeling lithium-ion solid-state electrolytes with a pinball model. Phys. Rev. Mater. 2, 65405 (2018)

MM 2.8 Mon 12:15 H44

Adaptive kinetic Monte Carlo driven by local environment recognition — ●KING CHUN LAI, SEBASTIAN MATERA, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Efficient lattice kinetic Monte Carlo (kMC) simulation generally relies on a complete prior-understanding of the possible elementary processes and their corresponding energy barriers. Adaptive kMC (akMC) overcomes this limitation by searching for those kinetics during the simulation, but the transition state searches (TSSs) become a bottleneck. To address this, we augment akMC with machine learning on local atomistic environments. Assigning a Smooth Overlap of Atomic Positions vector to each found process, we build up a database during simulation. This database is used to propose initial guesses for TSSs on basis of the proximity of the current local environments and the database entries. This proximity measure is self-adjusted based on statistics from TSSs on-the-fly. As the database fills, the proposed guesses from the database become close to the true transition states. These high quality TSS guesses improve simulation efficiency in two ways. First, the number of TSSs per kMC step gets significantly reduced by avoiding unsuccessful or repeating random TSSs. Second, damped Newton-Raphson becomes practical, which completes a proposed TSS in only a handful iterations. Taking a Pd surface as an illustrative example, we demonstrate the performance of the approach and also discuss how clustering and proximity learning can improve the TSS guesses further.

MM 2.9 Mon 12:30 H44

Atomistic Simulation Study of Li-Aluminosilicate Glass Scintillators — ●EL MEHDI GHARDI, PRINCE RAUTYAL, FIONA PEARCE, ANITA CROMPTON, LEE EVITS, SIMON MIDDLEBURGH, WILLIAM LEE, and MICHAEL RUSHTON — Nuclear Futures Institute, Bangor University, Gwynedd, LL57 2DG, United Kingdom

Radiation sensors are an important enabling technology in a number of fields, such as medicine, research, energy, military and homeland security. Glass base scintillators have been in use for more than 50 years and offer some benefits including their ability to respond to different types of radiation, and to be formed into various shapes. There is, however the possibility to discover and improve glass scintillators. With this in mind, this work provides insight from atomic scale simulations on the cerium doped Li-Aluminosilicate ($SiO_2 - Al_2O_3 - MgO - Li_2O - Ce_2O_3$) glass scintillators. Three glass compositions were studied using Molecular Dynamics (MD) and Density functional Theory (DFT) to investigate the effect of the ratio $R = ([Al_2O_3])/([MgO] + [Li_2O])$ (with $R = [0.3, 0.8 \text{ and } 2]$) on structural, electronic and optical properties. The effect of R on the complex structure of the system of interest was mainly associated to the increase of Q_4 population that replaced Q_3 's within the network, while electronic mid gap defects were found to be present when $R < 1$. The optical properties including absorption coefficients and energy loss spectra are calculated and analysed based on the electronic structures.

MM 2.10 Mon 12:45 H44

Bonding descriptor based approach for analysing and finding new Photovoltaic absorbers — ●JAKOB JOHANNES LÖTFERING and MATTHIAS WUTTIG — RWTH Aachen University, Aachen, Germany

The discovery of Halide Perovskites as good Photovoltaic absorbers and their rapid optimization lead to the question whether there are other materials yet undiscovered for Photovoltaic applications. In order to find new Photovoltaic absorbers, many approaches focus on structural data. We propose a bonding descriptor based approach using two quantities called electrons shared (ES) and electrons transferred (ET), which can be calculated using Density Functional Theory (DFT) calculations. ES and ET are derived from the Quantum Theory of Atoms in Molecules (QTAIM). The first quantity we employ is twice the delocalization index ($\delta(\Omega', \Omega)$) between neighboring atoms. The second one is the number of electrons transferred to/from an atom compared to the unbonded atom. $\delta(\Omega', \Omega)$ is a measure for the number of electron pairs shared between two atoms. It can be obtained by integrating the exchange-correlation pair density over two domains Ω and Ω' , which correspond to the two atoms. ES and ET have already shown to be good bonding descriptors and property predictors, e.g. for Halide Perovskites and Phase Change Materials. We propose that these quantities can also be used to analyse chemical bonding in Photovoltaic absorbers and predict novel materials in this category.

MM 3: Microstructures and Phase Transformations: Metals & Alloys

Time: Monday 10:15–12:45

Location: H45

MM 3.1 Mon 10:15 H45

Analysis of the precipitates in rapidly quenched Al-Cu alloys obtained in a magnetic pulse weld and through a melt spinning process — ●DAVID STEIN, MAXIMILIAN GNEDEL, and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, Universitätsstraße 1, 86159 Augsburg, Germany

Magnetic pulse welding (MPW) is a collision welding technique, where a flyer is accelerated towards a target using induced magnetic fields. This technique enables the welding of dissimilar metals. The microstructure of the interface is well described in the literature and typically displays a wave like structure. In the eye and wake of these waves an area of intermetallic phases can be found, depending on the materials and welding parameters. In this case an Al 1050 flyer and Cu DHP target were used. The structure of the interface has given strong indications of melting. Atomic resolution HAADF STEM was performed on this part and GP I and GP II Zones and disc shaped Θ' phases were found in the same area. The latter typically only form after longer heat treatments at elevated temperature. Albeit the theoretically predicted shape of Θ' Phases is disc shaped with very large diameter to thickness ratio, in the case studied here, they are much more compact and have a far smaller diameter to thickness ratio. The current working hypothesis is, that in the MPW process rapid solidification of the melt occurs, which leads to a high density of excess vacancies in the crystal structure, allowing for higher atom mobility. In an ongoing study we follow the precipitation process in rapidly quenched Al-Cu alloys obtained through a melt spinning process.

MM 3.2 Mon 10:30 H45

Crystal nucleation in undercooled Cu-Ge melts — ●MANOEL W. DA SILVA PINTO, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, WWU Münster

Experimental calorimetric data obtained by differential thermal analysis on the nucleation of undercooled Cu-Ge melts are presented. Deep undercooling levels have been reached throughout the entire composition range of this binary alloy in an experimental setup using an inorganic glass as an embedding medium. The heating and cooling cycles are statistically analyzed and lead to quantitatively determining nucleation rates independent of a specific nucleation kinetics model. Parameters of the classical nucleation theory, such as the kinetic prefactor and nucleation work, are extracted. We further discuss the data using different solution models for the alloy melts and consider their impact on nucleation kinetics. Thus, the nucleation kinetics parameters for the binary alloy system have been determined as a function of composition throughout the entire composition range and allow comparison with simplified models for concentration-dependent nucleation kinetics.

MM 3.3 Mon 10:45 H45

Experimental investigation of the early stage precipitation reactions in Al-Cu alloys — ●JOHANNES BERLIN, TOBIAS STEGMÜLLER, and FERDINAND HAIDER — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg

Due to their superior strength to weight ratio heat treatable Al-Cu alloys (2XXX-Series) are widely used particularly in aerospace industry. Although the hardening precipitates in these alloys are well-known, the very early stages of decomposition are still topic of ongoing research. Based on state-of-the-art scanning transmission electron microscopy, single Cu atoms can be imaged and natural ageing in form of Guinier*Preston zone formation accelerated by excess vacancies can be investigated, which was possible before only by diffraction experiments. Scanning transmission electron microscopy is used to investigate the influence of different parameters, such as thermal history, on early-stage precipitation in Al. The growth of GP I Zones is followed by ex-situ recording of a detailed time series during natural aging. In addition, resistivity 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 mechanisms leading to precipitate formation in these alloys for light-weight construction could be tuned more precisely regarding their intended use.

MM 3.4 Mon 11:00 H45

2D precipitate growth in a 3D matrix – Revealing the kinetics of Guinier–Preston zone formation in Al–Cu from atomic Monte Carlo — ●TOBIAS STEGMÜLLER and FERDINAND HAIDER — University of Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany

Guinier–Preston zones (GPZ) in Al–Cu, constituting the precipitate phase that was already responsible for the hardness increase in the first age-hardenable Al-alloy about 115 years ago, still attract attention first because of their special atomic mono- up to multilayer structure of Cu atoms and second due to their even at room temperature occurring formation, requiring an unexpected fast Cu diffusion.

To understand the origin of the GPZ structure, we performed Monte Carlo (MC) simulations mimicking precipitate growth by applying a Cluster Expansion (CE) for Al–Cu. From this we were able to identify an energy barrier above and below the layers of GPZ that is hardly overcome by migrating Cu. With this barrier we are able to explain the morphology of GPZ from a perspective focussing on the growth kinetics. On the one hand, the barrier guides migrating Cu to the layers' edges, supporting 2D growth. On the other hand, Cu atoms moving towards the layers' faces are stopped by the barrier, leading to nucleation of further Cu layers and explaining the multilayer shape.

To study the origin of the high Cu mobility, we recently included vacancies into simulations by switching from the CE based rigid lattice MC to a MC method allowing lattice relaxations by using a neural network interatomic potential. We present first results from this approach with regard to the interaction of vacancies with GPZ.

MM 3.5 Mon 11:15 H45

Atomic-scale observation of silver segregation in a high angle grain boundary in copper — ●LENA FROMMEYER, TOBIAS BRINK, GERHARD DEHM, and CHRISTIAN LIEBSCHER — Max-Planck-Str. 1, 40213 Düsseldorf

Although it is well recognized that segregation to grain boundaries (GBs) influences mechanical and electrical properties of materials, the impact of segregation on individual GB phases is poorly understood on the atomic level. Thermodynamic models are established to describe equilibrium segregation, but the atomistic origins and direct observation of solute segregation inside the GB core structure are seldomly investigated since high resolution imaging and spectroscopy are required.

Lately, we were able to resolve the atomic structure of a symmetric Σ 37c $\langle 111 \rangle$ {3 4 7} tilt GB in a Cu thin film using aberration-corrected high angle annular dark field scanning transmission electron microscopy (HAADF-STEM). By depositing a 100 nm thin Ag layer on top of our 2 μm -thick Cu thin film and subsequent annealing at 600°C, we could investigate the effect of Ag segregation on these GBs. Interestingly, the structure of the GB remains unchanged. Ag atoms solely substitute specific sites in the GB. If the Ag content in the GB is increased, one atomic column in the GB structure is filled up first, followed by four other columns. A combination of atomic resolution energy dispersive X-ray spectrometry, HAADF-STEM experiments and atomistic simulations were used to explore the underlying mechanisms leading to the observed Ag segregation pattern.

15 min. break

MM 3.6 Mon 11:45 H45

Grain boundary phase transitions and patterning in a copper tilt grain boundary — ●TOBIAS BRINK¹, LENA FROMMEYER¹, RODRIGO FREITAS², TIMOFEY FROLOV³, CHRISTIAN H. LIEBSCHER¹, and GERHARD DEHM¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Germany — ²MIT, USA — ³LLNL, USA

The atomic structure of grain boundaries (GBs) can exhibit different “phases” (also called complexions), which undergo thermodynamic phase transitions, but which have been observed in just a few simulation studies. Experimental confirmation often remains indirect. Here, we report on such a transition investigated by molecular dynamics computer simulations and supported by direct evidence from STEM imaging [1]. Two distinct atomistic structures could be found in a Σ 37c $\langle 111 \rangle$ tilt GB by a search with an evolutionary algorithm. Free energy calculations using the quasi-harmonic approximation predict a GB phase transition at 460 K. In the experiment, both phases also occur, but exhibit a pattern at room temperature in which the two

phases alternate. We present a hypothesis to explain this thermodynamically unexpected phenomenon by elastic interactions of the phase junctions, which are line defects with partial dislocation character.

Acknowledgment: This result is part of a project that has received funding from the ERC under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446).

[1] Frommeyer, Brink et al., "Dual phase patterning during a congruent grain boundary phase transition in elemental copper" Nat. Commun. (accepted, 2022)

MM 3.7 Mon 12:00 H45

Structural and thermal characterisation of a AuGe alloy via electron microscopy and fast differential scanning calorimetry — ●STEFAN STANKO¹, JÜRGEN SCHAWÉ^{1,2}, and JÖRG LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — ²Mettler-Toledo GmbH, Analytical, 8606 Nänikon, Switzerland

A device combining scanning electron microscopy (SEM) and fast differential scanning calorimetry (FDSC) was developed to perform *in situ* characterisation of metastable phase transformations. The potential of this device is demonstrated on the example of a AuGe eutectic alloy. Upon rapid cooling, the alloy forms the metastable crystalline phases β and γ and an amorphous phase. A thin lamella for transmission electron microscopy (TEM) was produced from a sample prepared in FDSC to further characterise the microstructure of the alloy beyond the capabilities of the *in situ* device. *Ex situ* FDSC experiments were performed using cooling and heating rates of several 1000 K/s to characterise the thermal behaviour of the β and γ phase. The transformation kinetics of the metastable phases was investigated. Finally, we show that we can prepare the glassy phase in FDSC and determine its thermophysical properties.

MM 3.8 Mon 12:15 H45

Phase decomposition in nanoporous Au-Pt — ●MAOWEN LIU^{1,2} and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Mechanics, Helmholtz-Zentrum Hereon — ²Institute of Materials Physics and Technology, Hamburg University of Technology

Nanostructured Au-Pt system has attracted great attention for its broad applications in catalysis. Due to the miscibility gap for a large

range of composition and temperature in bulk Au-Pt system, a comprehensive understanding of the structure transformation at various temperatures is necessitated. In the present work, nanoporous Au-Pt prepared by dealloying is selected for the investigation of the microstructure evolution during annealing. Dealloying transforms the homogeneous, ternary bulk solid solution Ag-Au-Pt into a nanoporous Au-Pt solution that would be immiscible at thermodynamic equilibrium. Remarkably, in view of the substantial atomic-scale rearrangement at the dissolution front, our experiments confirm a homogeneous Au-Pt solid solution. Upon annealing-induced coarsening, the phase structure evolves to semicoherent two-phase by way of an intermediate, coherent two-phase state.

MM 3.9 Mon 12:30 H45

Microstructural characteristics of lean magnesium alloys — ●TATIANA AKHMETSHINA, LEOPOLD BERGER, SAMUEL MONTIBELLER, ROBIN E. SCHÄUBLIN, and JÖRG F. LÖFFLER — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Lean magnesium alloys with less than 1 at.% of alloying elements are of high interest for biodegradable implant applications, where the implant remains only temporarily in the body, but degrades after it has fulfilled its task. With a specific combination of requirements, such as biocompatibility, appropriate mechanical properties and low degradation rate, such alloy development is still challenging. Here, we tailored the mechanical properties of lean Mg-Ca alloys by hot extrusion. The optimal alloying range was obtained via thermodynamic calculations using Pandat. The alloys were cast and extruded at the same ratio with different speeds and temperatures. A tensile toughness of up to 76 MJ/m³ was obtained, indicating a superior combination of strength and ductility. Depending on the extrusion parameters, the alloys exhibit a tensile strength of more than 420 MPa or, alternatively, a high ductility of up to 35% elongation at fracture. To obtain a clear understanding of the relationship between mechanical properties and microstructure, the latter was investigated by SEM, TEM and EBSD, focusing on precipitation, grain morphology, and dislocation structure. The grain size varied from submicrometer to several tens of micrometers. Apart from weak texture, the most ductile materials revealed an intriguing activation of $\langle c+a \rangle$ pyramidal slip.

MM 4: Structural Materials

Time: Monday 10:15–13:00

Location: H46

MM 4.1 Mon 10:15 H46

Nanoscale analysis of Ti-modified Mo-Si-B alloy to elucidate solid solution and particle strengthening — ●RESHMA SONKUSARE¹, TORBEN BOLL¹, JULIA BECKER², MARTIN HEILMAIER¹, and MANJA KRÜGER² — ¹Institute of Applied Materials and Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, Germany — ²Institut für Werkstoff- und Fügetechnik, Otto-von-Guericke-Universität Magdeburg, Germany

Mo-Si-B alloys are attractive high-temperature structural materials due to their high melting point (>2000C), high-temperature strength and good oxidation resistance. We found that small additions of Ti to multi-phase Mo-Si-B lead to strengthening of alloy at intermediate and high temperatures. To understand the effect of Ti on microstructure and thus mechanical properties, we investigated powder metallurgically processed Mo-7.2Si-9.7B-1.7Ti. The microstructure consists of Mo solid solution phase, intermetallic silicide phases, nanoscale oxide and silicide particles. To analyze the composition of these nanoscopic particles, atom probe tomography is required. APT reveals Ti to cause an unexpected compositional change of Mo(SS) phase. This change and an analysis of the composition and distribution of other phases combined with an investigation of the particles and elemental segregations at the grain boundaries and inside the grains improve the understanding of the solid solution and particle strengthening in the alloy and hence the mechanical behavior.

MM 4.2 Mon 10:30 H46

Intrinsic room temperature ductilisation of lean rare-earth free ternary Mg alloys — ●WASSILIOS DELIS¹, PIA HUCKFELDT¹, BENGT HALLSTEDT², PEI-LING SUN¹, DIERK RAABE³, SANDRA KORTE-KERZEL¹, and STEFANIE SANDLÖBES-HAUT¹ — ¹Institute for

Physical Metallurgy and Materials Physics, RWTH Aachen, 52074 Aachen, Germany — ²Institute for Materials Applications in Mechanical Engineering, RWTH Aachen, 52062 Aachen, Germany — ³Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Mg is a lightweight structural material with a good specific strength. Unfortunately, it lacks good room temperature formability and therefore a wider commercial use of Mg is hindered. The preferred basal slip and strong basal-type texture were found to be the main reasons for the poor room temperature formability. For basal slip the von Mises' criterion is not fulfilled. Recent experimental and simulative studies tried to activate more slip systems without changing the mechanical properties with alloying approaches. Alloys containing Y and rare-earth elements showed a highly increased room-temperature ductility. Since Y and rare-earth elements are costly further research has been carried out to identify similar acting alloy systems. For this purpose, the parameter I1 SFE has been used and the system Mg-Al-Ca was identified to have a similar I1 SFE. In experiments the system indeed showed the expected increased room temperature ductility. Further research of the effects of the chemical composition on the ductilisation has now been performed.

MM 4.3 Mon 10:45 H46

PT phase transitions and spectral structure of the interacting Hatano-Nelson model — ●SONGBO ZHANG — Stetthachrain 20, Zurich, Switzerland

In this talk, I will discuss the Hatano-Nelson model, i.e., a one-dimensional non-Hermitian chain of spinless fermions with nearest-neighbour nonreciprocal hopping, in the presence of repulsive nearest-neighbour interactions. At half-filling, I will show two PT transitions,

as the interaction strength increases. The first transition is marked by an exceptional point between the first and the second excited state in a finite-size system and is a first-order symmetry-breaking transition into a charge density wave regime. Persistent currents characteristic of the Hatano-Nelson model abruptly vanish at the transition. The second transition happens at a critical interaction strength that scales with the system size and can thus only be observed in finite-size systems. It is characterized by a collapse of all energy eigenvalues onto the real axis. I will also show that in a strong interaction regime, but away from half-filling, the many-body spectrum shows point gaps with nontrivial winding numbers, akin to the topological properties of the single-particle spectrum of the Hatano-Nelson chain.

MM 4.4 Mon 11:00 H46

Novel CDB Data Processing and Evaluation Software — ●LEON CHRYSOS, VASSILY VADIMOVITCH BURWITZ, LUCIAN MATHES, and CHRISTOPH HUGENSCHMIDT — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

The Coincidence Doppler-Broadening (CDB) spectrometer at NEPO-MUC has recently been upgraded with six additional HPGe Detectors, bringing the total number of detectors to ten. To take full advantage of the even more capable instrument a novel data evaluation software package (STACS) is currently under development. The software can already handle and visualize the data generated by Coincidence Doppler-Broadening Spectroscopy (CDBS) and provides a wide range of tools to analyze such data. Some of the main functions include the extraction of the electron-positron annihilation photo peak from CDB spectra as well as a simple background subtraction algorithm that is able to increase the peak-to-noise ratio of the extracted photo peak further. This combined with a new multi detector CDB function, which enables the combination of the data from all 10 detectors, provides detailed information about the chemical environment of the positron annihilation site. The software capabilities were tested on W samples, to demonstrate the sensitivity for high Doppler shifts. Measurements on the precipitation hardening properties of Al alloy samples were subsequently performed and will be shown.

MM 4.5 Mon 11:15 H46

Plasticity of the Ca(Al,Mg)₂ phase with variable temperature and composition — ●MARTINA FREUND¹, DOREEN ANDRE¹, PEI-LING SUN¹, NICOLAS J. PETER², and SANDRA KORT-KERZEL¹ — ¹Institut für Metallkunde und Materialphysik, RWTH Aachen University — ²Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Magnesium is a promising lightweight material, but its application as cast alloys at elevated temperature is limited because of its low creep resistance. By alloying with Al and Ca different Laves phases form, which improve creep strength. While investigating largely unknown properties with respect to composition and temperature changes, a challenge is to physically relate and represent such results. Here, we explore - in addition to the specific findings - how this may be done in terms of defect phase diagrams. Due to their complex packing, Laves phases are brittle at low temperatures. In order to overcome this restriction and to study their mechanical properties and mechanisms of plasticity, we used nanomechanical testing. For the cubic CaAl₂ phase, nanoindentation tests revealed a constant hardness of 5.9 ± 1.2 GPa and indentation modulus of 120.3 ± 17.9 GPa. Slip traces and cracks in the vicinity of indents were correlated with the crystal orientation and mostly corresponded to the {111} and {112} planes. Microcompression revealed deformation on {111} and {112} planes in <1-10> direction and the CRSS has been calculated as 0.97 ± 0.03 GPa and 0.96 ± 0.03 GPa, respectively. These planes and Burgers vectors were also confirmed by TEM using the g^{*}b criterion.

15 min. break

MM 4.6 Mon 11:45 H46

Ab initio study of magneto-chemo-structural coupling at FeMn grain boundaries — ●OMKAR HEGDE, JÖRG NEUGEBAUER, and TILMANN HICKEL — Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40227 Düsseldorf, Germany

Mn segregation at Fe grain boundaries is known to be a precursor for a variety of phenomena such as embrittlement, spinodal decomposition, phase transformation, etc [1,2]. Therefore, various heat treatments are performed in experiments to control Mn decoration at grain boundaries for *segregation engineering* [1], which could alter the lo-

cal magnetic state. In this direction, a thorough understanding of the connection between the local magnetic state and segregation remains elusive. In the present work, we tackle this issue by studying segregation in both the ferromagnetic state (low-temperature) and paramagnetic state (high-temperature) using ab initio-based approaches [3]. We demonstrate that the Mn segregation profile is mainly modulated by local magnetic interactions, providing new opportunities for grain boundary segregation engineering. Finally, we show that the formation of grain boundary and Mn segregation can, in turn, tune the local magnetic transition temperature, thereby revealing a complex coupling of structure, chemistry, and magnetism.

[1] D Raabe et al., Current Opinion in Solid State and Materials Science, 18, 253-261 (2014).

[2] AK Da Silva et al., Nature communications, 9, 1-11 (2018).

[3] O Hegde et al., Physical Review B, 102, 144101 (2020).

MM 4.7 Mon 12:00 H46

Sulphation kinetics of chloride particles, corrosion potential and effect of reactive additives — ●SEBASTIAN PENTZ and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, 86135 Augsburg

Chlorine induced high temperature corrosion leads to massive problems especially in waste-to-energy-plants, but also in biomass combustion. During the combustion process chloride containing particles are released and deposited on heat exchanger surfaces. There chlorides get converted into sulphates with a release of chlorine species which then lead to severe corrosion. In laboratory experiments we study the conversion kinetics under various conditions like temperature, particle size or gas composition. Both the sulphation reaction and the rate of subsequent corrosion show an Arrhenius dependency on temperature, a linear dependence on time, on particle surface and on partial pressure of SO₂. The addition of reactive additives can strongly influence this reaction and consequently the release of chlorine species: Adding iron oxide (e.g. Fe₂O₃) results in a strong acceleration of the sulphation process due to catalysis of the reaction from SO₂ to SO₃. On the other hand, a reduction of the sulphur content in the reaction atmosphere by desulphurising species like calcium oxide slows down the sulphation reaction and reduces the amount of released chlorine compounds. In lab experiments, chlorides (mixed with additives) are applied to 16Mo3 steel samples and exposed to a flowing reaction atmosphere in a tube furnace. Support by Federal Ministry for Economic Affairs and Climate Action on the basis of a decision by the German Bundestag.

MM 4.8 Mon 12:15 H46

Influence of oxygen and carbon on the chemistry at the niobium/alumina interface in a refractory composite material — ●MICHAEL EUSTERHOLZ¹, TORBEN BOLL¹, ALEXANDER KAUFFMANN¹, RESHMA SONKUSARE¹, VINCENT OTT¹, JULIAN GEBAUER¹, BASTIAN KRAFT¹, ANJA WEIDNER², MICHAEL STÜBER¹, SVEN ULRICH¹, and MARTIN HEILMAIER¹ — ¹Karlsruhe Institute of Technology (KIT) — ²TU Bergakademie Freiberg (TUBAF)

High-temperature processes such as steel casting impose harsh conditions on materials, which thus require excellent properties, including creep strength and resistance to thermal shock. Composites based on coarse-grained refractory metals and refractory ceramics promise superior performances due to adjustable mechanical and electrical properties.

Conventionally sintered composites from technical grade raw materials of α-Al₂O₃ and Nb include impurity elements that form carbides alongside oxides during synthesis. To understand the principles of formation, we investigate α-Al₂O₃ substrates sputter-coated with Nb as model materials beside the technical grade material. As the latter is subjected to carbon and oxygen containing gases during sintering, we compare the effect of oxygen and carbon overexposure on the ceramic-metal interface and contrast these results with a heat treatment with unaffected interface. Electron microscopy techniques elucidate the microstructure, while atom probe tomography advances the understanding of nano-scale phase formation at the phase boundary which are decisive for the material properties and corrosion resistance.

MM 4.9 Mon 12:30 H46

Oxidation mechanisms of SMART alloys and MAX phases — ●ANICHA REUBAN^{1,2}, JESUS GONZALEZ-JULIAN^{1,2}, IVAN POVSTUGAR¹, ANDREY LITNOVSKY^{1,3}, and CHRISTIAN LINSMEIER¹ — ¹Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — ²Institute of Mineral Engineering, RWTH Aachen University, 52064 Aachen, Germany — ³Moscow

Concentrated Solar Power (CSP) is a sustainable energy technology where sunlight is focused on a solar receiver and the thermal energy is used to generate electricity. The receiver must withstand temperatures greater than 1000 °C, be resistant to oxidation by air and/or corrosion by molten salts and maintain its properties over time. Self-passivating SMART alloys, originally designed for the fusion reactor, are resistant to plasma sputtering and can suppress oxidation in case of an accident with air ingress, up to 1000 °C. MAX phases, a bridge between metals and ceramics, are lightweight, easily machinable materials, oxidation- and corrosion-resistant up to 1400 °C. To understand the oxidation mechanisms in these materials, it is important to obtain nanoscale information using advanced characterization techniques such as Atom Probe Tomography (APT). According to the APT analysis of the SMART alloy W-Cr-Y, Y segregates at oxide grain boundaries while in the alloy it forms Y-O precipitates. Further analyses are being performed to get more information about the role of Y in the oxidation process. Electron microscopy is used along with APT for a correlative approach to nanoscale characterization.

MM 4.10 Mon 12:45 H46

Development of Tungsten fiber reinforced tungsten (Wf/W) using yarn based textile preforms — ●ALEXANDER LAU¹,

JAN WILLEM COENEN¹, DANIEL SCHWALENBERG¹, YIRAN MAO¹, ALEXIS TERRA¹, LEONARD RAUMANN^{1,2}, MICHAEL TREITZ^{1,4}, JOHANN RIESCH³, HANNS GIETL^{3,4}, BEATRIX GÖHTS¹, CHRISTIAN LINSMEIER¹, KATHARINA THEIS-BRÖHL², TILL HÖSCHEN³, and PHILLIP HUBER⁵ — ¹Forschungszentrum Jülich GmbH, Institut für Plasmaphysik, 52425 Jülich — ²Hochschule Bremerhaven, 27568 Bremerhaven — ³Max-Planck-Institute für Plasma Physics, 85748 Garching b. München — ⁴Technische Universität München, 85748 Garching — ⁵RWTH Aachen University, 52062 Aachen, Germany

The focus of this work is the development of a new composite material, that has to withstand the immense heat and particle fluxes in future fusion reactors. The wall material is based on the element tungsten, which already shows a very high compliance with the requirement profile in its pure form. Pure tungsten is inherently brittle below the DBTT and cracks could lead to a complete failure of the wall material. To counter this problem, extrinsic strengthening mechanisms were tested with new fabric types, based on radially braided yarns with seven core- and 16 sleeve filaments. These yarns were coated with an Yttriumoxide interface by Magnetron-sputtering and then further processed with chemically vapor deposited tungsten in a six-layer structure to form a solid composite material. This sample was analysed optically and got mechanically tested in a three-point bending test.

MM 5: Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 1

Time: Monday 15:00–15:30

Location: H44

Topical Talk

MM 5.1 Mon 15:00 H44

Vacancy transport in oxides exposed to high electric fields — ●REINER KIRCHHEIM — University of Goettingen, Goettingen, Germany — Max-Planck-Institute for Iron Research, Duesseldorf, Germany — I2CNER, Fukuoka, Japan

Internal electrochemical redox reactions and accumulation of charge in oxides are treated. Internal reactions shall lead to electronic conduction in the reduced and oxidized regions near cathode and anode respectively. Several scenarios for the generation and transport of charged oxygen vacancies and the attainment of steady state are discussed. It will be shown that at high cell voltages the characteristic

time for reaching steady state, also called incubation time, is smaller than the characteristic time for the growth of reacted regions. Then the incubation time is inverse proportional to the squared cell voltages or the voltage drop across the oxide, respectively. Examples were this relation is fulfilled are given for electromigration in integrated circuits, formation of memristors, flash sintering of ceramics and degradation of high-k materials. In addition, diffusion coefficients for vacancies evaluated from incubation times of yttria stabilized zirconia (YSZ) agree with extrapolated measured values. Internal reactions will also play a role in solid oxide fuel cell (SOFC) and solid oxide electrolysis cells (SOEC), where current densities may exceed the reaction rates with gases at the porous electrodes.

MM 6: Computational Materials Modelling: Defects / Alloys

Time: Monday 15:45–18:30

Location: H44

MM 6.1 Mon 15:45 H44

Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases — ●ZHUOCHENG XIE¹, DIMITRI CHAURAUD^{2,3}, ACHRAF ATILA^{2,3}, ERIK BITZEK^{2,3}, SANDRA KORTE-KERZEL¹, and JULIEN GUÉNOLE⁴ — ¹Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, 52056 Aachen, Germany — ²Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — ³Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — ⁴Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, 57070 Metz, France

In Laves phases, synchroshear is the dominant basal slip mechanism. It is accomplished by the glide of synchro-Shockley dislocations. However, the atomic-scale mechanisms of motion of such zonal dislocations are still not well understood. In this work, using atomistic simulations, two 30° synchro-Shockley dislocations with different Burgers vectors and core structures and energies are identified. We demonstrate that nucleation and propagation of kink pairs is the energetically favorable mechanism for the motion of the synchro-Shockley dislocation. Vacancy hopping and interstitial shuffling are identified as two key mechanisms related to kink propagation and we investigated how vacancies and antisite defects assist kink nucleation and propagation, which is crucial for kink mobility. These findings provide insights into the dependency on temperature and chemical composition of plastic deformation induced by zonal dislocations in topologically close-packed phases.

MM 6.2 Mon 16:00 H44

Macroscopic characteristics of plastic deformation described through dislocation mobility properties — ●SERGEI STARIKOV, ANTOINE KRAYCH, and MATOUS MROVEC — Ruhr University Bochum, ICAMS, Germany

Plastic deformation of bcc metals is a complicated phenomenon that links a behaviour of crystal defects with the macroscopic change of a sample shape. It is known that one of the basic mechanisms of plasticity is a motion of dislocations under applied stress. In this work, on the example of Mo and Nb, the study of plastic deformation in bcc metals was carried out with large-scale atomistic modelling. The temperature-dependent mobility functions of screw and edge dislocations were calculated from molecular dynamics simulation. The simulations of screw dislocation movement under applied shear stress revealed that the process can proceed in two different regimes: through thermally activated motion and athermal motion. Hence, the dislocation velocity depends on the shear stress in a non-trivial way. The calculated data provide a way to evaluate the basic macroscopic characteristics of plastic deformation at various temperatures and strain rates.

MM 6.3 Mon 16:15 H44

Analytic description of grain boundary segregation, tension, and formation energy in the copper–nickel system — TAMARA KRAUSS, FELIX FISCHER, and ●SEBASTIAN EICH — Institut für Materialwissenschaft — Lehrstuhl für Materialphysik, Universität Stuttgart
In this atomistic study, a recently proposed segregation model [1] is applied to segregation data of an exemplary $\Sigma 5$ grain boundary (GB), which is investigated using a copper–nickel embedded-atom method

potential. Segregation in the semi-grandcanonical ensemble is systematically studied by varying the chemical potential in order to explore the full composition range for temperatures from 500 K to 1000 K. As a major thermodynamic feature, the mentioned segregation model avoids the usage of *interface compositions*, for which an arbitrary volume must be defined, but rather models the thermodynamically unambiguous solute excess. It was shown that the solute excess and the interface formation energy could be described very accurately over a wide range of temperatures and over the entire composition. Since the model was initially derived for systems without lattice mismatch, the copper–nickel system with a mismatch of roughly 2.7% is chosen in this study to further extend the segregation model by a linear-elastic theory to also account for the interface tensions. Using this extended model, it will be shown that the solute excess, GB tensions, and GB formation energies can be derived from an effective energy of segregation for all temperatures and over the whole composition range [2].

[1] T. Krauß, S. M. Eich, *Acta Mater.* 187, 73 (2020)

[2] F. Fischer, S. M. Eich, *Acta Mater.* 201, 364 (2020)

MM 6.4 Mon 16:30 H44

Impurity segregation at grain boundaries in bcc iron: large scale models based on machine learned interatomic potentials — ●PETR ŠESTÁK¹, MONIKA VŠIANSKÁ^{1,2}, PAVEL LEJČEK^{1,3}, and MIROSLAV ČERNÝ¹ — ¹Central European Institute of Technology, CEITEC BUT, Brno University of Technology, Purkyňova 123, CZ-616 69 Brno, Czech Republic — ²Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 2, CZ-611 37 Brno, Czech Republic — ³Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, CZ-182 21 Prague 8, Czech Republic

In this work, we employed on the fly machine learning (ML) as it is implemented in the current version of the VASP to study segregation of Sn, P and Ge atoms at selected GBs (e.g. $\Sigma 3(112)$, $\Sigma 3(111)$, $\Sigma 5(310)$, $\Sigma 5(210)$, $\Sigma 13(510)$, $\Sigma 13(320)$, etc.) in bcc iron. Segregation energies were obtained using small supercells (<100 atoms), medium cells (~400 atoms) and also larger cells (>1000 atoms). Data obtained from the small and medium cells were compared with results of ab initio calculations as well as with available experimental data and predictions. This comparison serves as a benchmark of the interatomic potentials received from ML. The comparison shows that the segregation energies and some other GBs characteristics obtained for small cells are very consistent with ab initio simulations which bring a proof of reliability of interatomic potentials. The obtained results revealed that using small simulation cells (leading to high concentrations of impurity atoms), typical for ab initio simulations, might not be sufficient to predict correct segregation energies.

MM 6.5 Mon 16:45 H44

An efficient method to access the grain boundary parameter space with atomistic simulations — ●TIMO SCHMALOFSKI¹, MARTIN KROLL², REBECCA JANISCH¹, and HOLGER DETTE² — ¹ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany — ²Department of Mathematics, Ruhr-University Bochum, 44780 Bochum, Germany

A grain boundary (GB) is a two dimensional defect in solids with significant influence on different material properties. It describes the interface between two grains with different orientations and is thus defined by five macroscopic degrees of freedom (DOF), 2 from the rotation axis, 1 from the misorientation angle and 2 from the grain boundary normal vector. The GB energy as a function of the DOF can be obtained e.g. by atomistic simulations. However, a systematic sampling of the 5D grain boundary parameter space, or even lower-dimensional subspaces of it, comes with several challenges. To overcome them, a sampling method is needed, which only needs a small number of data points and can automatically find the cusps (deep minima) in the energy while sampling. Recently we introduced a sequential sampling technique which fulfills both [1] in the 1D subspace of symmetrical tilt grain boundaries. Now this sequential sampling technique will be evaluated for a 2D analysis of the energy as a function of GB plane inclination for fixed misorientations. [1] Kroll, M., Schmalofski, T., Dette, H. and Janisch, R. (2022), Efficient Prediction of Grain Boundary Energies from Atomistic Simulations via Sequential Design. *Adv. Theory Simul.* 2100615.

15 min. break

MM 6.6 Mon 17:15 H44

Electronic band gap of $\text{Al}_x\text{Sc}_{1-x}\text{N}$: a comparison of CPA and SQS — ●JAN M. WAACK^{1,2}, MARKUS KREMER^{1,2}, MICHAEL

CZERNER^{1,2}, and CHRISTIAN HEILIGER^{1,2} — ¹Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — ²Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Calculating physical properties of random substitutional solid solutions such as $\text{Al}_x\text{Sc}_{1-x}\text{N}$ requires specific methods such as the coherent potential approximation (CPA)[1] and special quasi-random structures (SQS)[2]. We compare the CPA in the framework of the atomic sphere approximation (ASA) Korringa-Kohn-Rostoker (KKR) density functional theory (DFT) with the SQS using the plane-wave pseudopotential DFT to calculate the lattice parameters and electronic band structures of the face-centered cubic phase of $\text{Al}_x\text{Sc}_{1-x}\text{N}$ (with $0 \leq x \leq 1$).

Using the low-computational-cost LDA-1/2 quasiparticle method[3] to calculate the electronic band structures within SQS and CPA, we present the first implementation of LDA-1/2 within the KKR DFT. We find that both the lattice parameter and the indirect band gap satisfy Vegard's law including a bowing parameter.

[1] C. Franz, M. Czerner, and C. Heiliger, *Phys. Rev. B* 88, 94421 (2013). <https://doi.org/10.1103/PhysRevB.88.094421>

[2] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, *Phys. Rev. Lett.* 65, 353 (1990). <https://doi.org/10.1103/PhysRevLett.65.353>

[3] L. G. Ferreira, M. Marques, and L. K. Teles, *Phys. Rev. B* 78, 125116 (2008). <https://doi.org/10.1103/PhysRevB.78.125116>

MM 6.7 Mon 17:30 H44

Using MD simulations to better understand and control self-propagating reactions in Al-Ni multilayers — ●FABIAN SCHWARZ and RALPH SPOLENAK — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

Reactive multilayers are capable of releasing large amounts of heat in a short time, making them a possible tool for energy storage or joining applications. Molecular Dynamics (MD) simulations can be used as a tool to study the front propagation, while varying certain system parameters. We study the influence of the crystal structure on the reaction front propagation in Al-Ni multilayers by looking at various microstructures, such as amorphous, single crystal or different grain structures. We found that crystallinity has a significant impact on the front propagation speed, which is likely related to different diffusion mechanisms. The more disordered the individual layers become, e.g., by increasing the grain boundary density, the higher is the resulting propagation speed. Furthermore, we study the influence of a premixed interlayer at the interface on the reaction propagation. For this, premixed interlayers with different, namely homogeneous, gradient and s-shaped profiles are studied and compared to existing experimental results. Beyond better understanding of the premixed interlayer, we show that it can be used to control the front propagation speed in reactive multilayers. Furthermore, we show that the heat of crystallization of amorphous AlNi to B2-AlNi alone is high enough for a self-propagating reaction to occur.

MM 6.8 Mon 17:45 H44

strong impact of spin fluctuations on the antiphase boundary energies of weak ferromagnetic Ni₃Al — ●XIANG XU^{1,2}, XI ZHANG², ANDREI RUBAN^{3,4}, SIEGFRIED SCHMAUDER¹, and BLAZEJ GRABOWSKI² — ¹Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart, Germany — ²Institute for Materials Science, University of Stuttgart, Germany — ³KTH Royal Institute of Technology, Stockholm, Sweden — ⁴Materials Center Leoben Forschung GmbH, Leoben, Austria

The antiphase boundary (APB) was believed to be crucial for explaining the anomalously increased yield stresses of L1₂ Ni₃Al. However, an accurate temperature-dependent APB energy is still missing and the magnetic effect was often underestimated or even neglected. In this work, the influence of longitudinal spin fluctuations (LSF) as well as other thermal mechanisms were considered within the ab-initio framework up till the melting point. We found that the calculated T-dependent APB energies show a remarkable agreement with the experimental data despite the large discrepancy between different works. The LSF effect was determined to crucially increase APB energies, especially for (100)APB with a maximum of 50% over the nonmagnetic data. This significant contribution prompts to take serious consideration of LSFs when studying the paramagnetism, even for weak itinerant ferromagnetic materials. The accurate APB energy acquired in this work can be used to set up quantitative models for simulating dislocation motions and the elastic-plastic behavior for Ni-based superalloys on the macro scale.

MM 6.9 Mon 18:00 H44

Ab initio study on the phase stabilities of multi-component carbides in high-Mn steels — LEKSHMI SREEKALA¹, JÖRG NEUGEBAUER¹, and TILMANN HICKEL^{1,2} — ¹Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — ²BAM Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

The high strength and ductility of advanced high Mn steels makes them suitable for lightweight applications in the transportation sector. A modification of their properties can be achieved by intentional or unintentional addition of further alloying elements, which is often connected with the formation of secondary phases. In particular, Cr addition improves corrosion resistance and, at the same time, inadvertently yields a substantial increase in the number of carbides precipitated, such as Fe₃C and Fe₂₃C₆. Therefore, in the present work, we use density functional theory to determine the thermodynamic driving force for the formation of these multicomponent carbides by evaluating their phase stabilities. We study the free energy of formation at finite temperatures by considering the vibrational, electronic and magnetic contributions. While both Cr and Mn stabilize Fe-carbides, we found that the impact of Cr is higher than that of Mn for a typical host matrix composition of Fe, Cr and Mn. Further, we analyze the critical role of magneto-structural coupling for the phase stability of these compositionally complex carbides. Through this study, we demonstrate the predictive capability of ab initio thermodynamics to accurately describe the phase stabilities of chemically complex secondary phases in metallic alloys.

MM 6.10 Mon 18:15 H44

Atomistic simulation of diffusion in γ' -strengthened Co-based superalloys — LIN QIN¹, JUTTA LOGAL^{2,3}, DOROTA KUBACKA⁴, and RALF DRATZ¹ — ¹ICAMS, Ruhr University Bochum, Bochum, Germany — ²Department of Chemistry, New York University, New York, United States — ³Department of Physics, Free University of Berlin, Berlin, Germany — ⁴Institute of Micro- and Nanostructure Research, FAU, Erlangen, Germany

The suppressed diffusion of Al in the strengthening γ' precipitates in Co-based superalloys is suspected to be one plausible reason to cause the selective formation of alumina in the early stage of oxidation above 900°C. In order to validate this assumption, the diffusion properties of Al, Co and W in a prototype structure of γ' phase, i.e. L1₂-Co₃(Al, W), are investigated with Density Functional Theory (DFT) and Kinetic Monte Carlo (KMC) simulations. DFT calculations reveal that the migration barrier of each element in Co sublattice is comparable with its respective barrier in pure Co. However, the crossover barriers of Al and W from their original positions to Co sublattice are much higher than the barriers for the reverse process. This large discrepancy in barriers constrains the site fraction of Al and W in Co sublattice, and therefore significantly suppresses the long-distance diffusion of Al and W in γ' phase. KMC results show that Al diffusivity in γ' phase is over two orders of magnitude lower than that in a solute γ phase (Co₇₅Al_{12.5}W_{12.5}) at 900°C, suggesting that the sluggish diffusion of Al in γ' can be a possible reason to cause the selective formation of alumina in Co-based superalloys.

MM 7: Microstructures and Phase Transformations: Oxides & Perovskites

Time: Monday 15:45–17:00

Location: H45

MM 7.1 Mon 15:45 H45

Evolution of a particle in twisted bilayer optical potentials — GANESH C. PAUL¹, PATRIK RECHER^{1,2}, and LUIS SANTOS³ — ¹Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany — ²Laboratory for Emerging Nanometrology, 38106 Braunschweig, Germany — ³Institut für Theoretische Physik, Leibniz Universität Hannover, Germany

Very recently few theoretical proposals have been put forward to simulate twisted bilayers using cold atoms in state-dependent optical lattices, which can be used as an alternative platform to investigate twisted bilayers in solid-state experiments. We study the band structure of both square and hexagonal geometries in an optical lattice setup, where the band structure can be tuned to be almost flat by proper implementation of interlayer Gaussian-type coupling. We examine the evolution of a particle in the twisted bilayer square-like potential, and find that the particle follows specific paths forming channels when the interlayer hopping is much stronger than the intralayer hopping strength. Due to the flexibility of controlling the inter- and intralayer coupling in optical lattices, our proposals should be easy to be realised in a cold atom set-up.

MM 7.2 Mon 16:00 H45

Phase transitions and phonon renormalization in CsPbBr₃ via a machine learning interatomic potential — ERIK FRANSSON¹, FREDRIK ERIKSSON¹, PETTER ROSANDER¹, TERUMASA TADANO², and PAUL ERHART¹ — ¹Chalmers University of Technology, Gothenburg, Sweden — ²National Institute for Materials Science, Tsukuba, Japan

Here, we present a study on phase-transition and phonon renormalization in the metal halide perovskite CsPbBr₃ using a machine learning (ML) interatomic potential. The ML potential is a neuroevolution-potential constructed using the GPUMD software and is trained on atomic forces, energies and stresses obtained from DFT calculations. We find that the ML potential captures the correct phase-transition from the orthorhombic phase to tetragonal phase and from tetragonal to cubic phase. The phase transition temperatures obtained are slightly underestimated compared to experimental studies, but in good qualitative agreement. These phase-transitions are connected to the so called tilt-modes at the R and M point in the Brillouin zone, which corresponds to tilting of the PbBr₆ octahedra. The dynamics of these modes are studied with MD simulations and mode projections, and we find that they have a strongly anharmonic and over-damped character. Furthermore, we investigate and benchmark how different

self-consistent phonon methods work for these strongly anharmonic modes.

MM 7.3 Mon 16:15 H45

A particular EFG temperature dependence for 181-Ta(TiO₂): An electron-gamma TDPAC study — IAN CHANG JIE YAP¹, JULIANA SCHELL^{2,3}, THIEN THANH DANG³, CORNELIA NOLL⁴, REINHARD BECK⁴, ULLI KÖSTER⁵, RONALDO MANSANO⁶, PETER BLÖCHL^{1,7}, and HANS CHRISTIAN HOFSSÄSS¹ — ¹Georg-August Universität Göttingen — ²European Organization for Nuclear Research (CERN) — ³Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — ⁴Helmholtz-Institut für Strahlen- und Kernphysik, University of Bonn — ⁵Institut Laue-Langevin — ⁶Escola Politécnica, Universidade de São Paulo — ⁷Technische Universität Clausthal, Institute of Theoretical Physics

In this work, we report on the hyperfine parameters of the implanted 181Ta probe in the rutile structure of the single crystal TiO₂ using the e - γ time differential perturbed angular correlation (e - γ TDPAC) technique. The experiments were performed under vacuum within the temperature range of 50 K - 427 K. The hyperfine parameters that are obtained from the e - γ TDPAC spectroscopy agrees with that of the γ - γ TDPAC spectroscopy at room temperature, apart from a calibration factor, both from our experiments and literature. Surprisingly, we have detected a parabolic increase of V_{zz} with a concave curvature at the low-temperature regime (50 K - 427 K), as opposed to the linear increase at the high-temperature regime (600 K - 1200 K) as found in the literature. Hence, we are performing DFT calculations on Ta-doped TiO₂ over a broad temperature range to obtain deeper insights.

MM 7.4 Mon 16:30 H45

Hidden charge order in square-lattice Sr₃Fe₂O₇ — DARREN C. PEETS^{1,2,3}, JUNG-HWA KIM¹, MANFRED REEHUIS⁴, PETER ADLER⁵, ANDREY MALJUK^{1,6}, TOBIAS RITSCHEL², MORGAN C. ALLISON², JOCHEN GECK^{2,7}, JOSE R. L. MARDEGAN⁸, PABLO J. BERECIARTUA PEREZ⁸, SONIA FRANCOUAL⁸, ANDREW C. WALTERS^{1,9}, THOMAS KELLER^{1,10}, PAULA M. ABDALA¹¹, PHILIP PATTISON^{11,12}, PINDER DOSANJH¹³, and BERNHARD KEIMER¹ — ¹MPI-FKF, 70569 Stuttgart — ²IFMP, TU Dresden, 01069 Dresden — ³NIMTE CAS, Ningbo, 315201 China — ⁴HZB, 14109 Berlin — ⁵MPI-CPFS, 01187 Dresden — ⁶IFW, 01171 Dresden — ⁷ct.qmat, TU Dresden, 01062 Dresden — ⁸DESY, Hamburg 22603 — ⁹Diamond, Didcot OX11 0DE, UK — ¹⁰MPI Outstation at MLZ, 85748 Garching — ¹¹SNBL at ESRF,

38042 Grenoble, France — ¹²EPFL, BSP-Dorigny, CH-1015 Lausanne, Switzerland — ¹³UBC, Vancouver, V6T 1Z1 Canada

Since the discovery of charge disproportionation in Sr₃Fe₂O₇ by Mössbauer spectroscopy >50 years ago, the spatial ordering pattern of the disproportionated charges has stayed “hidden” to conventional diffraction, despite numerous x-ray and neutron studies. Our neutron Larmor diffraction and Fe *K*-edge resonant x-ray scattering demonstrate checkerboard charge order in the FeO₂ planes that vanishes at a sharp second-order phase transition at 332 K. Stacking disorder of the checkerboard pattern due to frustrated interlayer interactions broadens their superstructure reflections, greatly reducing their amplitude, explaining the difficulty to detect them. We discuss implications of these findings for research on “hidden order” in other materials.

MM 7.5 Mon 16:45 H45

Band structure effects of a current-induced Mott-insulator to metal transition in Ca₂RuO₄ — ●D. CURCIO¹, C. E. SANDERS², A. CHIKINA¹, M. BIANCHI¹, H. E. LUND¹, V. GRANATA³, M. CANNAVACCIULO³, P. DUDIN⁴, J. AVILA⁴, C. POLLEY⁵, B. THIAGARAJAN⁵, A. VECCHIONE⁶, and P. HOFMANN¹ —

¹Department of Physics and Astronomy, Aarhus University, Denmark — ²STFC Central Laser Facility, Harwell Campus, United Kingdom — ³Dipartimento di Fisica *E.R. Caianiello*, Università degli Studi di Salerno, Italy — ⁴Synchrotron SOLEIL, Gif-sur-Yvette, France — ⁵MAX IV Laboratory, Lund University, Lund, Sweden — ⁶CNR-SPIN, c/o Università degli Studi di Salerno, Italy

The Mott insulator Ca₂RuO₄ can be turned into a metal by the application of a weak electric field and a corresponding transport current. This transition affects the optical and magnetic properties of the material. However, because of the electric field’s presence and the field-induced energy broadening, it is challenging to determine the electronic structure in the metallic state by angle-resolved photoemission spectroscopy (ARPES). Making use of the recently introduced approach to enable ARPES measurements of current-carrying devices by using a nano-scale light spot [1], we are able to measure ARPES data that tracks the current-induced phase transition in Ca₂RuO₄ simultaneously with the electrical transport, revealing the spectral function of the current-induced state along with a potential map of the sample’s surface.

[1] D. Curcio *et al.* Phys. Rev. Lett. 125, 236403 (2020).

MM 8: Materials for Storage and Conversion of Energy

Time: Monday 15:45–18:30

Location: H46

MM 8.1 Mon 15:45 H46

Atomistic analysis of Li migration in Li_{1+x}Al_xTi_{2-x}(PO₄)₃ (LATP) solid electrolytes — ●DANIEL PFALZGRAF^{1,2}, DANIEL MUTTER², DANIEL URBAN^{1,2}, and CHRISTIAN ELSÄSSER^{1,2} — ¹Freiburg Materials Research Center (FMF), University of Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg, Germany — ²Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

We present an examination of the ionic migration of Li in LATP [Li_{1+x}Al_xTi_{2-x}(PO₄)₃] solid electrolytes from an atomistic viewpoint based on density functional theory calculations [1]. In our study, we vary the Al content and investigate its effects on the crystal structure of LATP and on the migration energy landscape of interstitial Li ions. The energy profiles governing the Li diffusion are found to be systematically influenced by the position of Al ions in direct vicinity of the migration path, and we derive a simplified classification scheme of three universal energy profile shapes. The overall influence of the Al/Ti-ratio on the Li migration is analyzed by a separation into chemical and geometrical aspects. This work provides a solid basis for a resource-efficient computational examination of the ionic conductivity of Li in LATP with varying Al/Ti concentrations.

[1] D. Pfalzgraf, D. Mutter, and D.F. Urban, Solid State Ionics 359, 115521 (2021)

MM 8.2 Mon 16:00 H46

Diffraction tomography studies of lithium distribution in 18650-type Li-ion cells — ●ANATOLIY SENYSHYN¹, VLADISLAV KOCHETOV², DOMINIK PETZ³, and MARTIN MÜHLBAUER⁴ — ¹Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität Müncheng, Garching, Germany — ²Institut für Physik, Universität Rostock, Rostock, Germany — ³Physik Department, Technische Universität München, Garching, Germany — ⁴Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

At the moment Li-ion batteries are dominating in the segment of energy storage for portable electronics and electric drivetrains. Despite its overall popularity and widespread, the Li-ion technology has a high improvement potential, especially in the aspects concerning power and energy density, power fading, safety etc. Besides the variety of different factors, the chemical, mechanical and morphological uniformity of the cell components is one of the aspects crucial for optimization, estimation and prediction of cell parameters and cell behavior during standard operation and misuse. In the current contribution a series of diffraction-based methods (spatially resolved diffraction using radial oscillating collimators and/or conical slits as well as X-ray and neutron diffraction tomography) applied to probe inner structure of samples (either on example of dedicated phantom sample or cylindrical-type Li-ion battery) will be briefly introduced and reviewed.

MM 8.3 Mon 16:15 H46

Li diffusion in perovskite materials for battery applications

— ●WEI WEI¹, JULIAN GEBHARDT^{1,2}, DANIEL URBAN^{2,3}, and CHRISTIAN ELSÄSSER^{1,2,3} — ¹Cluster of Excellence livMatS, University of Freiburg, Germany — ²Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — ³Freiburg Materials Research Center (FMF), University of Freiburg, Germany

Metal halide perovskites are promising photovoltaic (PV) absorber materials, with the highest power conversion efficiency values currently exceeding 22%. Furthermore, unlike most of the traditional PV materials, hybrid perovskites have a strong ionic character. Therefore, these materials have recently been reported to have good ionic conductivity and lithium storage potential,^[1] allowing in principle the combination of a solar cell and a Li-ion battery in a single device. Here, we investigate this possibility by a Li-CsPbI₃ model system. By means of density-functional-theory calculations, we consider two scenarios: 1) Li in the rigid cubic perovskite structure, and 2) Li in the perovskite structure with flexible tilted bonds, which is the more realistic scenario at room temperature. The results of our simulations show that in the less symmetric structure the interstitial Li sites become nondegenerate and Li ions migrate along more complicated paths and have to overcome higher barriers than in the cubic structure. Nevertheless, diffusing Li ions have to overcome only moderate energy barriers of 0.16-0.33 eV, corroborating the potential use of metal-halide perovskites as Li-ion conducting PV materials.

[1] Zhen Li *et al.* Energy Environ. Sci.10 (2017) 1234

MM 8.4 Mon 16:30 H46

Analytical TEM studies of LiCoO₂ thin film electrode for Li-ion batteries — ●ARDAVAN MAKVANDI¹, SANDRA LOBE², MICHAEL WOLFF², MARTIN PETERLECHNER¹, CHRISTOPH GAMMER³, SVEN UHLENBRUCK², and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Institute of Energy and Climate Research, Materials Synthesis and Processing (IEK-1), Forschungszentrum Jülich GmbH, Jülich, Germany — ³Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

LiCoO₂ is the mostly used cathode material in commercial Li-ion batteries. However, only half of its theoretical capacity can be used due to the structural and chemical instability of its surface at charge voltages higher than 4.2 V. In general, interfaces (e.g. active material/coating, electrode surface/electrolyte) determine the local Li-ion transport kinetics and finally the electrochemical performance. 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 LiCoO₂ thin film before and after cycling are studied using transmission electron microscopy (TEM). In this case, the effect of an Al-doped ZnO-coating layer on the stability of the electrode surface upon cycling at high charge voltage has been studied.

MM 8.5 Mon 16:45 H46

Investigation of volume changes in the colquiriite structure due to Li insertion from first principles — ●ALJOSCHA BAUMANN^{1,2}, DANIEL MUTTER², DANIEL URBAN^{1,2}, and CHRISTIAN ELSÄSSER^{1,2} — ¹Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg — ²Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg

The long-term stability of lithium-ion batteries (LIB) is often negatively affected by mechanical stresses in the cathode material during charge/discharge cycles. Materials that show a zero-strain (ZS) behavior, i.e. their volume changes hardly during insertion or extraction of Li ions, are therefore of great interest. For individual compounds of the material class of colquiriites, $\text{LiA}^{\text{II}}\text{M}^{\text{III}}\text{F}_6$, ZS behavior has already been predicted theoretically and observed experimentally, e.g. for $\text{Li}_{1+x}\text{CaFeF}_6$, which exhibited a volume change of less than 0.5 % upon insertion of lithium ions up to $x=0.8$.

In order to identify the mechanism responsible for the ZS behavior we calculated the variation of the equilibrium volume due to varying Li concentration using density-functional theory (DFT). The analysis of the electronic and magnetic structure and local structure parameters at equilibrium volumes indicates that the total volume is influenced by a combination of expanding fluorine octahedra around the transition-metal ions due to the changing oxidation state, the distortion of octahedra around the Ca ions, and a decrease of repulsion between fluorine anions due to the inserted Li ions.

15 min. break

MM 8.6 Mon 17:15 H46

Cu₂+ Intercalated Vanadium Pentoxide Grown on Carbon Cloth as Binder-Free Cathodes for Reversible Aqueous Zinc Ion Batteries — ●PING HONG^{1,2}, YUDE WANG², HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²School of Materials Science and Engineering, Yunnan University, Kunming, People's Republic of China

Aqueous zinc batteries (ZIBs) with low cost, safety, environmentally friendly, and high theoretical capacity are a promising electrochemical energy storage technology. Vanadium based materials have been widely studied as cathode materials for ZIBs because of their safety, diverse crystal structure, abundant resources, low cost and high theoretical capacity. In the reported cathode materials, the mass loading of the cathode is usually less than 4 mg/cm² is not sufficient enough for practical applications. Herein, Cu₂+ intercalated vanadium pentoxide (CVOH@CC) with high loading (~7 mg/cm²) were directly grown on carbon cloth via hydrothermal method. The as-prepared CVOH@CC has a distinct 3D interconnected nested structure. When applying as binder-free cathode for ZIBs, CVOH@CC electrodes exhibited a high capacity of 223.4 mAh/g at 1.0 A/g and a long cycling performance of over 2000 cycles. The intercalation resulted in a better capacitive response and faster diffusion rate for the cathode compared to pure vanadium pentoxide (VOH@CC), which means better rate performance and cycling stability, providing a viable design proposal for the production of industrial grade ZIBs.

MM 8.7 Mon 17:30 H46

Reversible hybrid Na-CO₂ batteries with low charging voltage and long-life — ●CHANGFAN XU — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — School of Metallurgy and Environment, Central South University, Changsha 410083, China — Faculty of Metallurgical and Energy Engineering, Kunming University of Science and Technology, Kunming 650093, China

A reversible and long-life hybrid Na-CO₂ battery was proposed by using Na₃Zr₂Si₂PO₁₂ solid electrolyte as a separator, the saturated NaCl solution as an aqueous electrolyte, and nitrogen-rich graphitic carbon framework with well-defined morphology and dense bimetallic Fe-Cu sites (Fe-Cu-N-C) as cathodic catalyst. Besides having high Na⁺ ion conductivity, Na₃Zr₂Si₂PO₁₂ solid electrolyte also can prevent potential contamination from H₂O and CO₂ to sodium anode and avoid the internal short-circuit touch of Na dendrite with the cathode, thus improving the battery safety. The aqueous electrolyte can facilitate the dissolution of insulated discharge products, which overwhelmingly improves the reaction kinetics. The Fe-Cu-N-C cathodic catalyst can facilitate the fast evolution and degradation of flocculent discharge products. Finally, the hybrid Na-CO₂ battery exhibited an excellent

long-term cyclability with up to 1550 cycles (over 600 h). The reaction mechanism of Na-CO₂ battery was revealed by in-situ Raman, SEM and XRD analyses.

MM 8.8 Mon 17:45 H46

Revisiting the storage capacity limit of graphite battery anodes: spontaneous lithium overintercalation at ambient pressure — CRISTINA GROSU^{1,2}, ●CHIARA PANOSSETTI¹, STEFFEN MERZ², PETER JAKES², SEBASTIAN MATERA¹, RÜDIGER-A. EICHEL², JOSEF GRANWEHR², and CHRISTOPH SCHEURER¹ — ¹Fritz-Haber-Institut, Berlin, Germany — ²IEK-9, Forschungszentrum Jülich, Germany

The market quest for fast-charging, safe, long-lasting, and performant batteries drives the exploration of new energy storage materials, but also promotes fundamental investigations of those already widely used. Presently, revamped interest in anode materials is observed – primarily graphite electrodes for Li-ion batteries. We focus on the upper intercalation limit in the morphologically quasi-ideal highly oriented pyrolytic graphite (HOPG), with a LiC₆ stoichiometry corresponding to 100% state of charge (SOC). We prepared a sample by immersion in liquid lithium at ambient pressure. Investigation by static ⁷Li nuclear magnetic resonance (NMR) resolves unexpected signatures of superdense intercalation compounds, LiC_{6-x}. These were ruled out for decades, since the highest geometrically accessible composition, LiC₂, can only be prepared under high pressure. We thus challenge the widespread notion that any additional intercalation beyond LiC₆ is not possible under ambient conditions. We monitored the sample upon calendaric aging and employed *ab initio* calculations to rationalise the NMR results. The computed relative stabilities of different superdense configurations reveal that non-negligible overintercalation does proceed spontaneously beyond the currently accepted capacity limit.

MM 8.9 Mon 18:00 H46

The dielectric behaviour of Lithium intercalated graphite anodes as a function of the state of charge — ●SIMON ANNIÉS^{1,2}, CHIARA PANOSSETTI², MARIA VORONENKO¹, and CHRISTOPH SCHEURER² — ¹Theoretical Chemistry, Technical University Munich, Germany — ²Fritz Haber Institut, Berlin, Germany

The dielectric behaviour of battery materials is a crucial piece of information for understanding atomistic mechanics and modelling diffusion- and charging processes. However, for the most common anode material in today's Lithium ion batteries (Lithium intercalated graphite), literature results regarding this property are sparse, conflicting and only available for the empty state of charge (SOC).

Utilizing our recently developed DFTB parametrization (based on a machine-learned repulsive potential), we are - for the first time - able to compute the dielectric behaviour of Lithium intercalated graphite for the entire range of charge from 0% to 100%. Our results agree with experiments for 'empty' graphite, as well as for (bilayer-) graphene, which we use for an additional benchmark of our approach.

With increasing state of charge, we find a linear dependency of the dielectric constant, growing from around 7 at 0% SOC to around 29 at 100% SOC. With this, we lay an important piece of foundation for the understanding and multi-scale modelling of entire charging and discharging processes of Li-ion batteries.

MM 8.10 Mon 18:15 H46

In-situ analysis of SEI formation and cycle behavior on Sn by combined QCM-CV — ●KE WANG and GUIDO SCHMITZ — Chair of Materials Physics, Institute for Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany

Sn (Tin) could in principle be a promising candidate for a lithium-ion battery anode since it offers larger capacity than commercially graphite. But, researchers are still confused about the capacity fade especially caused by the formation of solid electrolyte interface (SEI). Here, we perform an in-situ characterization to clarify the mechanisms of SEI formation. Cyclic voltammetry has been conducted in combination with a quartz crystal microbalance to measure the growth of the SEI. Beside the overall mass increase, evaluating the mass change per charge (MPE) even enables identification of the ab/desorbed species. In advanced analysis, we combine three different characteristics including mass spectra, real-time MPE and average MPE, for the different stages of the long-term SEI formation. Except the SEI layer formed in first cycle, the SEI is continuously affected by the formation of Li₂O during lithiation and the oxidation of Sn during de-lithiation. In addition, the influence of the voltage window and the thickness of the electrodes on SEI formation are investigated. Remarkably, the SEI thickness reveals a linear relation to the electrode thickness which is

linked to continuous cracking and major oxidization of Sn bulk. Particularly, the inorganic part of the SEI formed during lithiation in the

specific voltage range of 0.36 - 0.27 V plays an important role on the microstructure of electrode and stabilizing the electrode.

MM 9: Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 2

Material modification

Time: Monday 17:15–18:30

Location: H45

Topical Talk

MM 9.1 Mon 17:15 H45

Design of corrosion-free and highly active electrocatalysts and photocatalysts via combinations of ab initio calculations and electrostatics — ●HEECHAE CHOI — Institute of Inorganic Chemistry, University of Cologne, Greinstr. 6, 50939, Cologne, Germany

Long enough lifetime of a catalyst is a very important, and frequently overlooked issue in catalyst design and development. For catalytic materials used in extreme conditions, corrosion resistance is the key factor to determine the lifetime and the steady performances over time. However, the theoretical design principle for the corrosion resistance of catalytic materials is lacking compared to the performance descriptor, which can give accurate predictions of catalytic activities of metallic materials. Recently, using the combinations of ab initio calculations and electrostatics model, we proposed a new theoretical scheme to improve the catalytic activity and corrosion resistivity. Under the hypothesis that the resistance of corrosion is a function of adsorption energy of corrosive ions in aqueous phases, we attempted to install built-in electric fields on heterogeneous catalyst surfaces. As the results, the performances of TiO₂ photoanode, Co/graphene Zn-air battery, and the water splitting by metal/carbon heterojunctions were highly improved. In this talk, I will introduce the procedures of such materials design theory developments and the experimental verifications.

MM 9.2 Mon 17:45 H45

Understanding DC-induced abnormal grain growth in FeC-thin films — ●THOMAS BREDE, MICHEL KUHFUSS, REINER KIRCHHEIM, and CYNTHIA VOLKERT — Institut für Materialphysik, Universität Göttingen, Deutschland

The field of processing materials with magnetic or electric fields and currents is steadily growing, since it opens the door to more efficient ways of material treatment and former not achievable material modifications. In this scope, it was shown recently, that high DC electric current densities up to 4 MA/cm² can be used at elevated temperatures of 550°C to produce elongated ferrite grains with high aspect ratios in an otherwise nanocrystalline iron-carbon thin film. To understand the underlying mechanism we will present experiments in a wide range of process parameters. The samples were characterized by SEM and EBSD in different stages of the experiment. The results shown allow a detailed description of the underlying mechanism of the evolution of the abnormal grown structures. In addition they reveal a threshold linked to the electromigration-induced C-flux, below which no changes occur. A purely kinetic model will be presented to describe the observed behaviour and allow the prediction of similar effects at

different process parameters and material systems.

MM 9.3 Mon 18:00 H45

Cavity induced and influenced phases of matter — ●CHRISTIAN J. ECKHARDT^{1,2}, GIACOMO PASSETTI², MARIOS MICHAEL¹, FRANK SCHLAWIN¹, DANTE M. KENNES^{2,1}, and MICHAEL A. SENTEF¹ — ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ²RWTH Aachen University, Aachen, Germany

An optical cavity may be used to influence or induce phases of matter. We discuss how a charge-density wave phase in a 1-dimensional chain of spinless fermions is enhanced through the coupling to the quantized photon field. At the critical point between the Luttinger liquid and the charge-density wave, we find strong light-matter entanglement. Additionally, we ask in what ways photons can be used as pairing glue for superconductivity (SC). We show that a fingerprint feature of such cavity-induced SC is the pickup of a k-dependence of the gap in the electronic spectrum on the Fermi-surface.

MM 9.4 Mon 18:15 H45

Floquet engineering the band structure of materials with optimal control theory — ●ALBERTO CASTRO^{1,2}, UMBERTO DE GIOVANNINI^{3,4}, SHUNSUKE SATO^{5,4}, HANNES HÜBENER⁴, and ANGEL RUBIO^{4,6} — ¹ARAID Foundation, Zaragoza (Spain) — ²Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza, Spain — ³Università degli Studi di Palermo, Dipartimento di Fisica e Chimica - Emilio Segrè, Palermo, Italy — ⁴Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ⁵Center for Computational Sciences, University of Tsukuba, Tsukuba, Japan — ⁶Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York NY

We demonstrate that the electronic structure of a material can be deformed into Floquet pseudo-bands with tailored shapes. We achieve this goal with a novel combination of quantum optimal control theory and Floquet engineering. We illustrate this framework utilizing a tight-binding description of graphene. We show several examples focusing on the region around the K (Dirac) point of the Brillouin zone: creation of a gap with opposing flat valence and conduction bands, creation of a gap with opposing concave symmetric valence and conduction bands, or closure of the gap when departing from a modified graphene model with a non-zero gap. We employ time periodic drives with several frequency components and polarizations, in contrast to the usual monochromatic fields, and use control theory to find the optimal amplitudes of each component that optimize the shape of the bands as desired.

MM 10: Poster Session 1

Time: Monday 18:00–20:00

Location: P2

MM 10.1 Mon 18:00 P2

Training Gaussian Approximation Potentials for Aqueous Systems — ●NIKHIL BAPAT, MARTIN VONDRÁK, JOHANNES T. MARGRAF, HENDRIK H. HEENEN, and KARSTEN REUTER — Fritz-Haber-Institut der MPG, Berlin, Germany

An accurate and efficient description of aqueous systems via atomistic computer simulations is of high relevance for many applications. Machine learning potentials (MLPs) trained on first principles data have demonstrated promising accuracy and computational efficiency for the length and time scales critical to the description of water. But even with the compelling advancements in MLPs, building a successful data-efficient atomistic model for complex aqueous systems remains a challenging task. The training of such MLPs can be notoriously difficult and so far required either negligence of chemical reactivity in the

MLP or excessive amounts of training data.

In this work we propose an efficient training procedure specifically designed for aqueous systems. To that end, we employ the widely applicable Gaussian approximation potential MLP and leverage it with a workflow for generating training data which ensures systematic inclusion of the bulk water configuration space. We calculate and compare ensemble properties of bulk water like its equilibrium density and diffusion coefficient to validate the MLP. The resulting model, when coupled with an added stimuli from a solid surface, can provide insights into many technologically important solid-liquid systems which are difficult to simulate otherwise.

MM 10.2 Mon 18:00 P2

Transfer learning on organic/inorganic interfaces for different substrates — ●ELIAS FÖSLEITNER, JOHANNES CARTUS, LUKAS HÖR-

MANN, and OLIVER T. HOFMANN — Graz University of Technology, Graz, Austria

Performing structure search of organic molecules on metallic surfaces requires finding the structure with the lowest energy. Using conventional density functional codes this proves to be a time-consuming task, since the number of possible configurations is large and individual calculations are expensive. For all-electron approaches, this becomes even more problematic when calculating molecules on metal substrates of higher nuclear charge number, e.g. on gold. To circumvent the computation of all possible configurations, machine learning techniques such as Gaussian process regression proved to be a useful tool to reduce the amount of calculated data.

In our work we further reduce the data requirements by using transfer learning from one substrate to another. To this end, we first train the system on substrate A, and use this information to accelerate the learning process of the system on another substrate B. This is done by using the energy predictions of substrate A as a prior for the machine learning model imposed on system B. By doing so, we can reduce the data requirements for the training of expensive systems to an extent that makes the investigation computationally feasible.

MM 10.3 Mon 18:00 P2

Large-scale molecular dynamics simulations using fourth generation neural network potentials — ●EMIR KOCER¹, ANDREAS SINGRABER², TSZ WAI KO¹, JONAS FINKLER³, PHILIPP MISOF², CHRISTOPH DELLAGO², and JÖRG BEHLER¹ — ¹Georg-August University, Göttingen, Germany — ²University of Wien, Vienna, Austria — ³University of Basel, Basel, Switzerland

In the last decade, their proven success in bridging the gap between ab initio and classical molecular dynamics made machine learning potentials (MLP) very attractive. However, many MLPs are short-ranged and unable to capture interactions beyond a certain cutoff, which leads to inaccurate forces and energies in systems where long-range interactions are important. While MLPs including long-range electrostatic interactions based on local charges have been available for some years, only recently fourth generation MLPs have emerged that can take also global phenomena like non-local charge transfer into account. An example is the fourth generation high dimensional neural network potential (4G-HDNNP), which utilizes a global charge equilibration step. This study presents a modified version of 4G-HDNNPs, in which the matrix solution is replaced by a function minimization algorithm for an enhanced scalability on multi-core systems. The new potential has been implemented into the LAMMPS software and tested in large-scale molecular dynamics simulations.

MM 10.4 Mon 18:00 P2

Interatomic Potential Fitting in pyiron — ●MARVIN POUL¹, NIKLAS LEIMERO², ALEXANDER KNOLL³, MARIUS HERBOLD³, and JOERG NEUGEBAUER¹ — ¹Max-Planck-Institut fuer Eisenforschung — ²Universitaet Goettingen — ³TU Darmstadt

Interatomic potentials have a key role in computational materials science bridging the gap between Ab-Initio methods and large-scale engineering applications. pyiron[1] is an IDE for computational materials science that allows for reproducible yet easy to write simulation protocols. Within its framework we have developed tools that allow for semi-automatic fitting and verifying of potentials. This includes wrappers for AtomicRex[2] (for classical potentials) and as well the machine-learned Moment Tensor Potentials (MTP[3]), high-dimensional neural network potentials (HDNNP[4]), and ACE potentials. In this work we introduce the facilities offered by our code on the examples of an Magnesium MTP and an EAM potential for Copper.

[1]: <https://doi.org/10.1016/j.commatsci.2018.07.043>

[2]: <https://doi.org/10.1088/1361-651X/aa6ecf>

[3]: <https://doi.org/10.1088/2632-2153/abc9fe>

[4]: <https://doi.org/10.1103/PhysRevLett.98.146401>

MM 10.5 Mon 18:00 P2

Effect of temperature pre-treatments on atomic dynamics in PdNiP studied with ECM — ●OLIVIA VAERST, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Material Physics, University of Münster, Germany

Pre-treatments on amorphous PdNiP, such as annealing and treatments of thermo-mechanical kind, significantly influence the local structure, kinetic stability, and mechanical properties of this bulk metallic glass (BMG).

In the present work, Pd₄₀Ni₄₀P₂₀ samples are pre-treated thermally

by annealing them at different temperatures below the glass transition temperature. The resulting well-defined states are investigated via transmission electron microscopy (TEM) with electron correlation microscopy (ECM) at room temperature. ECM is used to study atomic rearrangements and dynamics in the material at nanometer spatial resolution [1,2]. The effect of thermal pre-treatments on ECM evaluation parameters is discussed. Such investigations of the atomic mobility in pre-treated PdNiP give further insight into underlying mechanisms and properties of the amorphous phase as well as on the local relaxation dynamics of a bulk metallic glass.

[1] L. He et al., *Microsc. and Microanal.* 21 (2015) 1026-1033.

[2] K. Spangenberg et al., *Adv. Funct. Mater.* 31 (2021) 2103742.

MM 10.6 Mon 18:00 P2

Investigating the short-range order of amorphous GeTe upon structural relaxation obtained by TEM diffractometry and RMC methods — ●CHRISTIAN STENZ¹, JULIAN PRIES¹, T. WESLEY SURTA², MICHAEL W. GAULTOIS², and MATTHIAS WUTTIG¹ — ¹Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany. — ²Faculty of Chemistry, University of Liverpool, Liverpool L7 3NY, United Kingdom.

New experimental insights into the structural changes during resistance drift in amorphous GeTe are presented. Selected area electron diffraction is performed on a-GeTe in five different annealing states to compute the pair distribution functions upon relaxation. Examination of the short-range order based on the order parameters $S(q_2)/S(q_1)$ and r_2/r_1 implies a continuous increase in the most prominent average bond angle by 1° towards 104.5°. This is consistent with the analysis of the bond angle distribution (RMC simulations) which reveals a shift of the main contribution ($\sim 103.5^\circ$) towards larger angles. A concomitant increase of intermediate geometries between tetrah. and octah. ($\sim 140^\circ$) is observed. Applying three different techniques to estimate the fraction of tetrahedral Ge atoms the three measures coherently suggest a decrease in tetrahedrality. We conclude that an enhancement of Peierls-like distorted/pyramidal motifs, *i.e.* an increase in the PD -ratio r_L/r_S , causes the increase of the average bond angle, resulting in a widening of the band gap. This structural relaxation ultimately leads to the resistance drift.

MM 10.7 Mon 18:00 P2

Influence of swift heavy ion irradiation on Pd-based metallic glasses — ●SABA KHADEMOREZAIAN¹, MAXIMILLIAN DEMMING¹, MARILENA TOMUT^{1,2}, SERGIY DIVINSKI¹, and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — ²GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

Bulk and ribbon samples of Pd₄₀Ni₄₀P₂₀ in as-quenched and relaxed states were room-temperature irradiated with 4.8 MeV/u 179Au ions at the UNILAC accelerator. Ion beam-induced surface patterning associated with irradiation masks and smoothening of the surface were studied by laser scanning microscope and profilometry. Irradiation induces an out-of-plane swelling step of approximately 100 nm as measured at the boundary between the irradiated and non-irradiated areas and can be explained by additional free volume creation in the solidified ion tracks. The swelling and plastic flow mechanisms are analyzed. Changes in the relaxation enthalpy have been investigated using differential scanning calorimetry. Low-temperature heat capacity measurements substantiate prominent irradiation-induced changes of the Boson peak. Furthermore, changes in diffusivity with increasing fluence was found by post-irradiation tracer diffusion measurements. The evolution of mechanical properties was probed by nanoindentation measurements and the changes induced by irradiation are compared with those caused by mechanical rejuvenation.

MM 10.8 Mon 18:00 P2

Investigations on the relaxation of metallic glasses using fast scanning calorimetry — ●MAXIMILIAN DEMMING, MARK STRINGE, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, 48149 Münster

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. In this work different relaxation states achieved by in-situ quenching via FSC are examined and compared to the relaxation behavior observed at conventional rates.

MM 10.9 Mon 18:00 P2

Investigation of thermoelectric transport through infrared spectroscopy of Heusler and Heusler-like compounds based on Fe₂VAl — ●SAHRA BLACK, MICHAEL PARZER, FABIAN GARMROUDI, ERNST BAUER, ANDREI PIMENOV, and EVAN CONSTABLE — Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

Thermoelectric materials have attracted much interest in recent years for their ability to convert a thermal gradient into an electric current, thereby acting as an electric power generator. Full and half Heusler compounds have attracted special interest in the growing field of thermoelectricity for several members with a high thermoelectric performance. One Heusler compound in particular Fe₂VAl was under investigation for its high power Factor PF and its high thermoelectric figure of merit ZT . And recently the element doped thin film Fe₂V_{0.8}W_{0.2}Al broke the world record for the highest thermoelectric figure of merit of roughly 5 ever recorded.

The purpose of the project was to investigate the dielectric response of the thermoelectric material class Fe₂VAl under different manufacturing methods with the usage of Fourier-transformed infrared (FTIR) spectroscopy. This led to a better understanding of the different contribution to the thermoelectric figure of merit ZT .

MM 10.10 Mon 18:00 P2

Atom probe tomography study of diffusion in Al-TiB₂ and Al₃Ta-TiB₂ systems — ●EVGENIA VOLOBUEVA, PATRICK STENDER, JIEHUA LI, and GUIDO SCHMITZ — University of Stuttgart, Institute of Material Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

To improve the quality of castings, grain refinement is a technique that can improve the overall qualities and properties of the material. For grain refinement in aluminum casting processes, TiB₂ and Ta are added. It is well known, that Al and Ta form an Al₃Ta phase inside the Al-based alloy. In order to gain insight into the process of grain refinement, the diffusion of Al₃Ta and Al in TiB₂ crystals was analyzed via Atom Probe Tomography (APT) in detail.

In this project, single crystals of TiB₂ were used as raw material, glued on top of tungsten posts. Both pure aluminum layers and stoichiometric Al₃Ta layers were deposited by sputter deposition on these crystals with a layer thickness of 200 nm. Subsequent annealing treatments were carried out to investigate segregation and diffusion phenomena at the crystal interface. To use the high spatial and chemical resolution of APT, the samples were sharpened to a final apex radius of 50 nm by azimuthal milling using a Focused Ion Beam Instrument (FIB). Observed segregation and determined diffusion coefficients will be presented.

MM 10.11 Mon 18:00 P2

Highly conductive Graphite Intercalated Compounds — ●LEONHARD NIEMANN — Robert Bosch GmbH

Since its discovery, graphene has been a material of great research interest due to its promising properties of high electron mobility and electrical conductivity. However, the proposed applications have not yet been realized due to the complexity of fabricating high-quality, defect-free, large-area graphene films. Graphite, which consists of stacked graphene layers, does not have the same promising properties but is easier to fabricate. By intercalating Lewis acids between the graphene layers of graphite, the layers decouple and graphene like behaviour is achieved. The conductivity of these graphite intercalated compounds (GIC) is increased. Here, we report a gas-phase intercalation method for graphite films with AlCl₃, resulting in GICs with 20 MS/m. These films exhibit good long-term thermal stability. It is noted that the final conductivity depends on the electrical conductivity of the un-

treated graphite films which is affected by defects in single graphene flakes and the flake size. Studies to increase the conductivity of non-intercalated graphite films are necessary to increase the conductivity of GICs. Therefore, further studies on graphenization of graphite films and defect healing are conducted and the results are presented.

MM 10.12 Mon 18:00 P2

Flatbands and Nonlinear Transport in Nodal Line Semimetals — ●THOMAS BÖMERICH, JINHONG PARK, and ACHIM ROSCH — Institute for Theoretical Physics, University of Cologne, Germany

Ohm's law describes the linear dependence of the current on the electric field. Although deviations from this relation are quite small for usual metals we present a model of a semimetal with large non-ohmic conductivity. Motivated by recent experiments on ZrTe₅ we study a low-energy Hamiltonian consisting of a single Dirac point which gets deformed into a nodal line by mirror symmetry breaking. Upon Landau quantization a zero energy state for a wide range of momenta emerges. For small densities the lowest Landau level can be reached at feasible magnetic fields making it possible to investigate the properties of the flatband.

While flatbands have generated growing interest because of their large density of states and the importance of interactions, we instead focus on their impact on nonlinear transport. Using the Boltzmann equation we obtain higher order conductivities and compare our results to a Dirac semimetal. We show that in the quantum limit, the nonlinear signal of the nodal line semimetal is five orders of magnitude larger than the Dirac semimetal. This enhancement of the nonlinear properties originates from the emergence of the flat bands in the nodal line semimetal. Additionally we investigate the influence of disorder on the linear conductivity.

MM 10.13 Mon 18:00 P2

Towards an efficient formalism to calculate Electron-Phonon-coupling Self Energies and Transport properties from MD Simulation — ●MARKUS KREMER^{1,2}, MICHAEL CZERNER^{1,2}, and CHRISTIAN HEILIGER^{1,2} — ¹Institut für Theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — ²Zentrum für Materialforschung Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Calculating transport properties for finite temperature systems has been a concern of research for a long time, with the semiclassical Lowest-order-variational approximation to the Boltzmann-equation (LOVA) being the most commonly used. Recently it was presented that within the KKR formalism more accurate results can be obtained for some materials by using a quantum mechanical Landauer-Büttiker approach incorporating phase-breaking scattering.

Here we want to investigate the possibility of obtaining transport properties at finite temperatures by using a classical MD Simulation and carrying out a transport calculation in the KKR formalism of a certain amount of randomly picked MD screenshots. This procedure is repeated for different lengths of the device to verify that the cell shows ohmic behaviour and obtain its specific resistance. Afterwards we can map this specific resistance to a self-energy.

MM 10.14 Mon 18:00 P2

Determination of interdiffusion coefficients for Pt-Pd binary system by Atom Probe Tomography and DFT calculations — ●YOONHEE LEE¹, XI ZHANG², SEBASTIAN MANUEL EICH¹, PATRICK STENDER¹, BLAZEJ GRABOWSKI², and GUIDO SCHMITZ¹ — ¹Department for Materials Physics, Institute for Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²Department of Materials Design, Institute for Materials Science, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Understanding the diffusion behavior of different alloy components is fundamental and many systems are well evaluated with distinct diffusivities. However, despite its significant usage as a catalyst for many applications, the interdiffusion behavior of the Pt-Pd binary system has not yet been fully uncovered due to the remarkably slow atomic migration. In this work, interdiffusion coefficients have been determined from experimental data and compared with the results of DFT simulations. For the temperature range between 400 and 700 °C, nano-sized multilayer samples were created by Ion-Beam Sputtering (IBS). After heat treatment, the samples are analyzed by Atom Probe Tomography (APT). Obtained composition profiles are fitted by a Fourier series approach and the respective interdiffusion coefficients are determined. For the temperature range between 800 and 970 °C, micron-sized Pt/Pd diffusion couples are used and analyzed using EDX. The

respective interdiffusion coefficients are determined by the Boltzmann-Matano method. All interdiffusion coefficients are compared with DFT simulations.

MM 10.15 Mon 18:00 P2

Imbibition- and Drying-Induced deformation of Nanoporous Solids — ●JUAN SANCHEZ¹, PATRICK HUBER¹, HOWARD STONE², LARS DAMMANN¹, and ZHUOQUING LI¹ — ¹Hamburg University of Technology (TUHH), Hamburg, Germany — ²Princeton University, NJ, USA

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (Vycor glass) upon spontaneous, capillarity-driven infiltration of water as well as drying. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformation originating in changes in the surface stress at the inner pore walls (dynamic Bangham's regime), whereas the second results from Laplace pressure effects. The interplay of both strain-inducing regimes allows to infer the water content in the pore space.

The theoretical framework used to describe our experimental data combines simple continuum mechanics and fluid dynamics on the macroscopic porous-solid scale, supported by molecular dynamics simulations on the single-nanopore scale. Our study demonstrates that it is possible to monitor imbibition and drying dynamics by simple dilatometry measurements, offering multiple potential applications.

MM 10.16 Mon 18:00 P2

The Interplay of Spreading, Imbibition and Evaporation of Droplets at Nanoporous Surfaces — ●LAURA GALLARDO^{1,2,3}, JUAN SÁNCHEZ^{1,2,3}, OLIVIER VINCENT⁴, and PATRICK HUBER^{1,2,3} — ¹Institute for Materials and X-Ray Physics, Hamburg University of Technology, 21073 Hamburg, Germany — ²Center for X-Ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — ³Center for Hybrid Nanostructures CHyN, University of Hamburg, 22607 Hamburg, Germany — ⁴CNRS & Univ. Lyon 1, Institute for Light and Matter (ILM), Villeurbanne, France

The dynamics of a droplet deposited on a porous substrate is a combination of three phenomena: spreading, imbibition and evaporation. Here we present a study on the interactions of droplets on nanoporous silicon prepared by electrochemical etching as a function of time. The evolution of the droplet volume is analyzed theoretically and experimentally considering the evaporation and the imbibition of the liquid into the porous substrate. Water is employed to illustrate the case of an evaporation-dominated regime [1]. For an imbibition-dominated regime squalane is employed. The very low vapor pressure of this fluid allows for the analysis of the imbibition process of a droplet into a porous substrate without the contribution of evaporation. The agreement between the experimental data and the theoretical predictions deepens the understanding of the structure of HF-etched porous silicon substrates and provides new insights into the fundamentals of fluid transport in nanoporous media.

[1] Seker, Erkin, et al. APL 92.1 (2008): 013128

MM 10.17 Mon 18:00 P2

Kinetic trapping in brittle crack opening — ●TOBIAS MÜLLER and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

In the 1920s, Griffith introduced his continuum approach for fracture. Since then great efforts were made to describe crack propagation more precisely within continuum mechanics. Nevertheless, it is evident that the atomic structure of the crack tip itself plays a major role in crack advancement, thus making it necessary to extend the concept of Griffith to the discrete atomic level. This enables the possibility to investigate essential and material-specific processes, such as local bond rearrangements and path-dependent activation barriers. In general, crack opening is a complex chemical process on a multi-dimensional potential energy surface with many local minima and saddle points. The complexity even increases if parameters such as temperature, pressure or chemical environments are included. Here we discuss first DFT-based geometry optimizations for silicon to study brittle fracture mechanics. We show that cracks can propagate via a multitude of local energy minimum configurations connected by a variety of energy barriers. We highlight the complex nature of crack advancement and the complexity of modelling and finding the correct fracture pathway even for a material with a simple crystal structure such as silicon.

MM 10.18 Mon 18:00 P2

Comparison of Crack - Dislocation Interactions in fcc and bcc Metals — ●BENEDIKT EGGLE-SIEVERS and ERIK BITZEK — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The Interactions between Cracks and Dislocations are investigated by means of large scale atomistic simulations with EAM-potentials. Dislocations of different character and Burgers vector are placed in the vicinity of a strain-controlled crack, resulting either in an attraction or repulsion of the dislocation. In the former case further interactions can be observed in the course of the simulation, e.g. dislocation emission or crossslipping of screw parts. Dependencies on the stress state, the crack system, dislocation character and distance between dislocation and crack tip are investigated in fcc and bcc crystals. The results are discussed in the framework of resolved shear stresses acting on the dislocations in the near field of the crack tip and for different dislocations characteristics in fcc and bcc.

MM 10.19 Mon 18:00 P2

Molecular dynamics analysis of point defects in ferroelectrics — ●TAKAHIRO TSUZUKI¹, DILSHOD DURDIEV², FRANK WENDLER², RYO KOBAYASHI¹, MASAYUKI URANAGASE¹, HIKARU AZUMA¹, and SHUJI OGATA¹ — ¹Nagoya Institute of Technology, Nagoya, Japan — ²Friedrich-Alexander University of Erlangen-Nürnberg, Fürth, Germany

Ferroelectrics are used in many devices such as capacitors. Pb(Zr, Ti)O₃ is the most used material in piezoelectric devices but it contains lead which is gradually prohibited using these days because lead is poisonous to human health. BaTiO₃, which is a very famous classical ferroelectric and lead-free, is newly focused on because its characteristics improve treated by containing defects. But the mechanism of the effects of the defects is not well understood.

We investigated the effects of point defects, monovacancies, and first and second neighbor divacancies on the domain growth of BaTiO₃ with an applied electric field by molecular dynamics simulation using core-shell inter-atomic potential. We found that the first neighbor Ba-O divacancy is the most effective on the domain growth [1]. The sum of the electric field from the divacancy dipole and applied electric field, when they are in the same direction, strongly assist the domain growth.

Phase-field models are powerful tools to investigate ferroelectrics in mesoscale simulation. We obtained parameters, which contain the effect of vacancies mentioned above, for a phase-field model from the molecular dynamics simulation.

[1] Tsuzuki T. et al., J. Appl. Phys. 131, 194101(2022).

MM 10.20 Mon 18:00 P2

Effect of increasing Mn content on generalized planar fault energies of Ni-Mn-Ga alloys — ●MARTIN HEČZKO¹, PETR ŠESTÁK², and MARTIN ZELENÝ¹ — ¹Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — ²Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

Giant magnetic field induced strain (MFIS) in martensitic phase of Ni-Mn-Ga ferromagnetic shape memory alloy makes this alloy promising for various applications. The reasons for existence of MFIS are the high mobility of twin boundaries combined with large magneto-crystalline anisotropy. We performed our calculations using the spin-polarized DFT method implemented in the Vienna Ab Initio Simulation Package (VASP) to reveal the effect of increasing concentration of excess Mn on formation and propagation of twin boundaries, which can be characterized by changes in generalized planar fault energy (GPFE) curves. Effects of excess Mn local arrangement in Ga sublattice on GPFE curves has been considered as well.

Our results show that the barriers for nucleation and grow of a twin rise with increasing content of Mn. It results in more difficult twin formation and propagation in compositions far from stoichiometry. This effect is even more enhanced if excess Mn atom in Ga sublattice is located exactly in the planar fault.

MM 10.21 Mon 18:00 P2

Influence of Twin Boundaries on the Mechanical Behavior of Nanowires Subjected to Bending — ●SABA KHADIVIANAZAR^{1,2}, JONAS SCHICKEL¹, and ERIK BITZEK^{1,2} — ¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Chair of General Materials Properties, Institute I, Martensstr. 5, Erlangen 91058, Germany — ²Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf 40237, Germany

Metallic nanowires (NWs) display superior mechanical properties compared to their bulk counterparts and are regarded as promising building blocks for a variety of application such as touchscreen displays, flexible and stretchable electronic devices. Recently it has been observed that the multi twinned nanowires show higher yield stress and enhanced localized deformation compared to the single crystalline nanowires. Despite the importance of characterizing the deformation behavior under bending loads, most studies of metallic twinned NWs to date have been performed under tensile testing conditions.

Here we present recent results of atomistic simulations on bi-crystalline twinned nanowires under bending. Atomistic simulations allow for controlled variation of the material, size, morphology, the location of the twin boundary (TB), and loading conditions. We show that the presence of a TB not only influences the plastic deformation but also affects the stress state of nanowires. The critical resolved shear stress for dislocation nucleation was determined and the interactions of dislocations with TBs was studied in detail for varying twin boundary location and bending directions.

MM 10.22 Mon 18:00 P2

Benchmarking a Machine-Learning Enhanced Dimer Method for Transition State Search — ●NILS GÖNNHEIMER, KING CHUN LAI, KARSTEN REUTER, and JOHANNES T. MARGRAF — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The implementation of Machine-Learning (ML) surrogate models into established atomistic simulation types (e.g. molecular dynamics or geometry optimizations) offers the opportunity of significantly lowering their computational cost. The Dimer method for finding saddle points on high-dimensional potential surfaces is a prime example of this. This method is an important tool for locating transition states and exploring reaction mechanisms in heterogeneous catalysis, but applications are limited by its large computational cost. Jacobsen et al. recently showed that this can be overcome by combining Dimer search with a Gaussian Process Regression surrogate model in the Artificial Intelligence-Driven dimer (AID-TS) algorithm. To better understand the role of the ML surrogate in this method, we compare accuracy, efficiency and diversity of the found states, for AID-TS and conventional dimer search, using surface self-diffusion of Pd(100) as an example.

MM 10.23 Mon 18:00 P2

Al-Ge solid solubility prediction using machine-learned force-field potentials and phonon calculations — ●ONDŘEJ FIKAR and MARTIN ZELENÝ — Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

This work is focused on a theoretical study of the phase stability of Al rich solid solution in Al-Ge alloy. The solubilities of the solid solution were first determined using temperature-dependent free energies of pure elements and solid solutions of various chemical compositions obtained from ab initio calculations based on density functional theory. All total energy calculations were performed by Vienna Ab initio Simulation Package (VASP) with the help of Projector Augmented-wave potentials. Contributions of vibrational free energy and electron free energy were obtained from Phonopy package. Subsequently, a forcefield potential for Al-Ge alloy using machine learning routines as implemented in the VASP package was created. The trained forcefield potential was then used to again carry out phonon calculations. The results were compared to the previous phonon calculations carried out without machine learning.

MM 10.24 Mon 18:00 P2

Simulation of long-term diffusion-based processes in Al and Ni — ●DARIA SMIRNOVA¹ and ERIK BITZEK^{1,2} — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The study of coupled diffusive-displacive processes like dislocation climb at the atomic scale is inherently challenging due to the vastly different time scales involved in the individual processes. One way to address this challenge is to extend the possible simulation timescales while keeping proper atomistic description of a system by using diffusive molecular dynamics (DMD). The method combines classical atomistic interaction potentials in the variational Gaussian method with a numerical solver for the diffusion equation on a variable grid given by the atom positions. Recently, various computational implementations of DMD were presented. Here we describe in detail the different implementations of DMD and provide benchmarks for their efficiency using vacancy diffusion at defects in Al and Ni as model systems.

MM 10.25 Mon 18:00 P2

Ab initio study on novel precipitate-matrix interfaces in Al-Sc based alloys — ●UJJAL SAIKIA¹, TILMANN HICKEL^{1,2}, SANKARAN SHANMUGAM³, SERGIY V. DIVINSKI⁴, and GERHARD WILDE⁴ — ¹Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH — ²BAM Bundesanstalt für Materialforschung und -prüfung — ³Indian Institute of Technology Madras — ⁴Institute of Materials Physics, University of Münster

The cube-on-cube orientation relationship (OR) with the Al matrix has been accepted as the orientation relationship for the coherent nano-scaled Al₃Sc-based particles in Al. Recently, in a severely cold-rolled and subsequently annealed Al-Sc-Zr-Ti alloy, atomic-scale investigations using high resolution scanning transmission electron microscopy (HRSTEM) reveals a novel type of precipitate/matrix coherency.

We performed density functional theory (DFT) based total energy calculations to understand the mechanism of formation of this new type of precipitate/matrix coherency between Al₃Sc and Al matrix and to compare it with the established interfaces. Our DFT results reveal that the newly observed interface corresponds to a local minimum of energy and there is an energy penalty for the interface boundary to ‘escape’ the particle. We also studied segregation behavior of Sc atoms to probe the initial stage of formation of the observed novel Al₃Sc/Al interface.

MM 10.26 Mon 18:00 P2

Ab initio study of point defects in disordered systems — ●PAVEL PAPEZ¹, MARTIN FRIÁK², and MARTIN ZELENÝ¹ — ¹Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — ²Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, Czech Republic

This work is focused on a theoretical study of the influence of N and C interstitials in the equiatomic medium entropy alloy CoCrNi. These interstitials can be found in the alloy as contamination after preparation by powder-metallurgy techniques. The study was done by employing ab initio calculations based on the density functional theory and was performed by Vienna Ab initio Simulation Package (VASP) using the projector-augmented-wave formalism. The calculations were done on 6x6x2 supercells generated by using the special quasi-random structures approach (SQS) consisting of 216 atoms. The supercell consisted of 6 lattice planes {1 1 1} along the z-axis. The hcp structures were made from the fcc cells by moving the planes to create the hcp ABABAB stacking. Our results have shown which interstitial positions result in the lower enthalpy of formation. They are characterized by a higher amount of Cr and lower amount of Ni in their nearest neighbours (NN) shell with the most stable being the one with 2 Co, 3 Cr, and 1 Ni in its 1st NN shell. The stacking fault energy (SFE) was calculated using the first-order axial Ising model and by explicit stacking-fault calculations in two times larger fcc supercell. The results shown that interstitials always increase the SFE.

MM 10.27 Mon 18:00 P2

Charge distribution and electronic structure of ZIF-8 and its derivatives from first principles — ●JOSHUA EDZARDS¹, HOLGER-DIETRICH SASSNICK¹, ANA MARIA VALENCIA^{1,2} und CATERINA COCCHI^{1,2} — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg — ²Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin

Metal organic frameworks are novel materials with high potential in many fields of applications, ranging from gas storage and catalysis to optoelectronics. In spite of their growing popularity, there is still a lack of fundamental understanding of the physico-chemical properties of these materials, even in the most established subgroups such as the zeolitic imidazolate frameworks (ZIFs). To shed light into the nature of the chemical bonds in these systems, we performed a first-principles study based on density-functional theory investigating the charge distribution in ZIF-8 and its derivatives with Br, Cl, and H terminations replacing CH₃. Our results indicate the presence of an ionic bond connecting the Zn atom to the organic scaffold, which is held together by covalent bonds. Control calculations performed on the building blocks of ZIF-8 indicate that the aforementioned characteristics are quantitatively influenced by the extended nature of the framework. The presence of halogen substituents, carrying around an excess of negative charge, leads only to a negligible redistribution of the charge density. On the other hand, the electronic structures computed for these systems indicate a reduction of about 0.5 eV of the

band-gap in the Br- and Cl-terminated systems with respect to ZIF-8.

MM 10.28 Mon 18:00 P2

Recent progress in ICET — J. MAGNUS RAHM, •ERIK FRANS-SON, PERNILLA EKBORG-TANNER, JOAKIM BRORSSON, MATTIAS ÅNGQVIST, and PAUL ERHART — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Alloy cluster expansions (CEs) provide an accurate and computationally efficient mapping of the potential energy surface of multi-component systems that enables comprehensive sampling of the many-dimensional configuration space. In this contribution, we provide an update regarding recent developments and new features in the integrated cluster expansion toolkit (ICET). We have implemented a version of the constituent strain formalism in ICET, which enables treatment of long-ranged strain contributions. This approach is demonstrated for the Pd-H system in order to study coherent phase transitions via constrained Monte Carlo simulations. Furthermore, in CEs of low-dimensional systems, lack of symmetry leads to large numbers of independent effective cluster interactions (ECIs). We have made it possible to merge orbits, i.e., reduce the number of independent ECIs by considering local symmetries and merging parameters that are similar. This approach enables training of accurate models while requiring significantly fewer DFT calculations. This approach is employed to study surface segregation in AuPd and CuPd in environments ranging from vacuum to high pressures of hydrogen. Finally, we have added a number of additional features, including Wang-Landau sampling and extraction of long-range order parameters, and the code has undergone a thorough review that has resulted in a significant performance boost.

MM 10.29 Mon 18:00 P2

Molecular dynamics simulations of porous silica networks — •HEMANGI PATEL¹, BARBARA MILOW^{1,2}, and AMEYA REGE¹ — ¹Institut für Werkstoff-Forschung, Abteilung Aerogele und Aerogelverbundwerkstoffe, Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Cologne, Germany — ²Nanostructured Cellular Materials, Institut of Inorganic Chemistry, University of Cologne, Cologne, Germany

Molecular dynamics (MD) simulations offer a significant advantage

over experimental procedures to investigate the nanoporous structure in silica-based systems because they present a detailed insight into the atomic-scale phenomena that underlie the formation of the materials* network. In this work, porous silica networks are modelled using MD simulations. α - quartz form of SiO₂ is subjected to high temperature and equilibration followed by quenching to obtain amorphous silica structure α - quartz form of SiO₂ is subjected to high temperature and equilibration followed by quenching to obtain amorphous silica structure. The negative pressure rupturing approach is then used to obtain a fractal structure. Local minimum energy configuration is obtained using the conjugate gradient scheme for the formation of a stable porous network. The structural evolution of the silica backbone in the network is investigated. This technique is used to obtain porous networks of varying densities. The resulting model systems are investigated for their structural and mechanical properties. Uniaxial tensile and compressive simulations will be presented, and properties such as their Young's modulus will be quantified.

MM 10.30 Mon 18:00 P2

Magnetotransport properties of coupled nanowire arrays in LAO/STO — •RANJANI RAMACHANDRAN¹, DENGYU YANG¹, MUQING YU¹, ADITI NETHWEWALA¹, PATRICK IRVIN¹, JEREMY LEVY¹, and KI-TAE EOM² — ¹University of Pittsburgh, Pittsburgh, USA — ²University of Wisconsin-Madison, Madison, WI, USA

The ability to create and characterise an array of coupled nanowires is an important step towards understanding the physics of systems like stripe phase superconductors, sliding Luttinger liquids, anisotropic materials made up of quasi-1D chains, etc. Here, we create nanowire arrays using Ultra Low voltage Electron beam lithography. ULVEBL has been shown to create conducting nanostructures in the 2D electron system at the LAO/STO interface. We study the transport properties of this system at low temperatures and high magnetic fields. We show that it is possible to reversibly tune the interwire coupling using a back gate voltage and magnetic field. This can act as a tool to study the dimensionality cross over from 1D to 2D. This can potentially be extended further to create more complicated structures using ULV-EBL that can model the behaviour of other materials and lattice models.

MM 11: Invited Talk Jörg F. Löffler

Time: Tuesday 9:30–10:00

Location: H44

Invited Talk

MM 11.1 Tue 9:30 H44

Fast calorimetry: studying phase transitions in slow motion — •JÖRG F. LÖFFLER — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 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 fast calorimetry to slowly transforming BMG-forming systems at heating and cooling rates of several 10,000 K/s, we are able to determine phase transitions more or less in slow motion. In this way, we can explore novel glass states [1], determine their stochastics of nucleation, and study metastable phase formation. During heating at low tem-

peratures, BMGs generally form metastable crystals that transform into more stable modifications at higher temperatures. The classical interpretation is a direct solid-to-solid transformation, but by fast calorimetry we can show that this transition occurs via metastable melting [2]. Furthermore, while with classical calorimetry it is not possible to sufficiently characterize metastable phases owing to their structural changes upon slow heating, fast calorimetry allows for detailed measurements of their heat capacity and melting temperatures [3]. In this way, we are able to verify the existence of monotropic polymorphism and validate Ostwald's phase rule for many metastable phases. [1] J. E. K. Schawe, J. F. Löffler, Nat. Commun. 10, 1337 (2019). [2] S. Pogatscher et al., Nat. Commun. 7, 11113 (2016). [3] J. E. K. Schawe, J. F. Löffler, Acta Mater. 226, 117630 (2022).

MM 12: Computational Materials Modelling: Physics of Ensembles 1

Time: Tuesday 10:15–13:00

Location: H44

MM 12.1 Tue 10:15 H44

Pinpointing Hubbard corrections to tackle inhomogeneous n_l subshells: The DFT+U(m) method — ●ERIC MACKE¹, IURI TIMROV², LUCIO COLOMBI CIACCHI¹, and NICOLA MARZARI² — ¹Hybrid Materials Interfaces Group and Bremen Center for Computational Materials Science, MAPEX, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany — ²Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

DFT+U remains a key tool in computational material science as it mitigates the DFT self-interaction error. While this simplistic approach often provides electronic and magnetic properties in fair agreement with literature, recent investigations revealed that DFT+U massively over-stabilizes high spin configurations of transition metal elements surrounded by strong ligand fields. In such compounds, the projection of occupied Kohn-Sham states onto the atomic basis frequently yields occupation numbers $n_m^\sigma \approx 0.5$ for certain magnetic quantum numbers m , so that the penalizing Hubbard term $E_U = \sum_{m,\sigma} \frac{U}{2} [n_m^\sigma (1 - n_m^\sigma)]$ is maximized. We argue that if the occupation of a magnetic (spin-) orbital is dominated by the effect of hybridization with a ligand, Hubbard corrections should not be applied in the same way as for unaffected orbitals. To account for such inhomogeneous bonding regimes, we propose a more flexible scheme that enables the use of distinct Hubbard parameters $U(m)$ for the same species, computable by means of *ab initio* methods.

MM 12.2 Tue 10:30 H44

Efficient computation of optical properties of large-scale heterogeneous systems — ●JOSEPH C. A. PRENTICE¹ and ARASH A. MOSTOFI² — ¹Department of Materials, University of Oxford, UK — ²Departments of Physics and Materials, Imperial College London, UK

The optical properties of large-scale (>1000 atoms) heterogeneous systems are of interest in several fields, from photovoltaics to biological systems. Computing such properties accurately from first principles, however, is challenging; even if only a small region is optically active, quantum mechanical environmental effects must often be included, and the cost of applying a quantitatively accurate level of theory is prohibitive. Here, I present recent work demonstrating how such calculations can be performed efficiently from first principles via two methods: an extension of the spectral warping method of Ge et al., and a novel combination of quantum embedding (specifically embedded mean-field theory) and linear-scaling (time-dependent) density functional theory. The accuracy and utility of these methods is demonstrated by applying them to systems including the molecular crystal ROY, chromophores in solution, and pentacene-doped p-terphenyl. The results pave the way for quantitatively accurate calculations to be performed on previously inaccessible large-scale systems.

MM 12.3 Tue 10:45 H44

Converging tetrahedron method calculations for non-dissipative parts of spectral functions — ●MINSU GHIM^{1,2,3} and CHEOL-HWAN PARK^{1,2,3} — ¹Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — ²Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — ³Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Integrations in k space are used to calculate many of the physical quantities in solid-state physics. Examples include various static or dynamical conductivity, self-energy of an electron, and electric polarizability. The integral usually takes the form of a product of proper matrix elements and $1/[\hbar\omega - (\epsilon_{m\mathbf{k}} - \epsilon_{n\mathbf{k}}) + i\eta]$, which is decomposed into the real part and the imaginary part, $\text{P}\{1/[\hbar\omega - (\epsilon_{m\mathbf{k}} - \epsilon_{n\mathbf{k}})]\}$ and $-i\pi\delta[\hbar\omega - (\epsilon_{m\mathbf{k}} - \epsilon_{n\mathbf{k}})]$, respectively. Here, ω is the frequency, $\epsilon_{m\mathbf{k}}$ and $\epsilon_{n\mathbf{k}}$ are the energies of the valence and conduction electronic bands with Bloch wavevector \mathbf{k} , respectively, and $\eta = 0^+$. Although the delta-function part has been widely calculated by the tetrahedron method, the non-dissipative principal value integral part has not. Tools to obtain matrix elements and energy eigenvalues from first principles have been actively developed, but there are technical difficulties in the tetrahedron method for the non-dissipative part. In this talk, we introduce an easy-to-implement, stable method to overcome those ob-

stacles. Furthermore, our method is tested by calculating the spin Hall conductivity of fcc platinum.

MM 12.4 Tue 11:00 H44

Self-consistency in GWT formalism leading to quasiparticle-quasiparticle couplings — ●CARLOS MEJUTO-ZAERA¹ and VOJTĚCH VLČEK² — ¹Scuola Internazionale Superiore di Studi Avanzati SISSA, Trieste, Italy — ²University of California Santa Barbara UCSB, USA

Many-body perturbation theory (MBPT) has become a tool of choice for the description of materials. Traditionally tied to the weakly-interacting limit, e.g. through the GW approximation, its expansion towards higher interactions is a fundamental goal in the field. Existing attempts can rely on selected diagram resummation or downfolding, which involve some choice of expansion parameters typically reducing the approach's generality and flexibility. Despite this apparently intrinsic price, MBPT provides through Hedin's equations a formally exact path to describe any dynamically correlated system, regardless of interaction strength. We revisit this framework to disentangle how to systematically extend its practical validity beyond weak interactions, focusing on the structure of the interaction vertex Γ within self-consistent implementations. Using the Hubbard dimer at half-filling, we unveil the role of Γ 's functional derivative with respect to the Green's function, hitherto typically neglected, in generating diagrams that can extend the reliability of MBPT towards high interactions [1].

[1] arXiv:2203.05029

MM 12.5 Tue 11:15 H44

Automated Corrections for Materials Design of Ionic Systems: AFLOW-CCE — ●RICO FRIEDRICH^{1,2}, MARCO ESTERS¹, COREY OSES¹, STUART KI¹, MAXWELL J. BRENNER¹, DAVID HICKS¹, MICHAEL J. MEHL¹, CORMAC TOHER¹, and STEFANO CURTAROLO^{1,3} — ¹Center for Autonomous Materials Design, Duke University, USA — ²Helmholtz-Zentrum Dresden-Rossendorf, Dresden — ³Materials Science, Electrical Engineering, and Physics, Duke University, USA

Materials databases such as AFLOW [1] leverage *ab initio* calculations for autonomous materials design. The predictive power critically relies on accurate formation enthalpies — quantifying the thermodynamic stability of a system. For ionic materials such as oxides and nitrides, standard 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]. Here, we introduce AFLOW-CCE [4] — our implementation of CCE into the AFLOW framework. It provides a tool where users can input a structure file and receive the CCE corrections, or even the CCE formation enthalpies if pre-calculated LDA, PBE or SCAN values are provided. The implementation features a command line tool, a web interface, and a Python environment.

[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).[4] R. Friedrich *et al.*, *Phys. Rev. Mater.* **5**, 043803 (2021).

15 min. break

MM 12.6 Tue 11:45 H44

Revealing the ambient and high-pressure phases of group IV monochalcogenides and monoxides with an evolutionary algorithm — ●LONG NGUYEN and GUY MAKOV — Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel

Group IV chalcogenides and oxides are candidates for incorporation into optoelectronic and thermoelectric conversion devices. These functional materials are mostly p-type semiconductors that provide low-cost, environmentally friendly, abundant, and high-efficiency. To expand the possible phases and study their stability upon compression, a combination of DFT modelling with evolutionary algorithm (EA) is applied to extensively investigate across the group IV monochalcogenides and oxides. We will report our results from the implementation of the EA to search for stable phases. In group IV monoxides, our results include multiple structural transitions of SnO and PbO upon

compression. Two new high-pressure polymorphs are predicted, the orthorhombic Pbcm SnO and the octahedral monoclinic C2/m PbO. Weakening of the lone pairs and elastic instability are the main drivers for the structural transitions. Among the monochalcogenides, SnS and GeS phase families are examined together with their electronic and optical properties. At ambient conditions, GeS and SnS can present several polymorphs with bandgaps in the range from 0.3 to 1.6 eV, which can be attractive for a variety of optoelectronics applications. Upon compression, we found a similar convergence of SnS and GeS into the Cmcm and later the Pm3m phase. The transition mechanism is discussed through the lone pairs' influence on the structural distortion.

MM 12.7 Tue 12:00 H44

An Open-source Interface to MP2 and Coupled-Cluster Methods for Solids for Localized Basis Set Codes — ●EVGENY MOERMAN¹, FELIX HUMMEL², ANDREAS IRMLER², ANDREAS GRÜNEIS², and MATTHIAS SCHEFFLER¹ — ¹The NOMAD Laboratory at the FHI-MPG, Berlin — ²Inst. for Th. Phys., TU Wien, Vienna

Coupled cluster (CC) theory is often considered the gold standard of quantum-chemistry. For solids, however, the available software is scarce ([1] and references therein). We present CC-aims[2], which can interface ab initio codes with localized atomic orbitals and the CC for solids (CC4S) code by the group of A. Grüneis. CC4S features a continuously growing selection of wave function-based methods including perturbation and CC theory. The CC-aims interface was developed for the FHI-aims code[2] but is implemented such that other codes may use it as a starting point for corresponding interfaces. As CC4S offers treatment of both molecular and periodic systems, the CC-aims interface is a valuable tool, where DFT is either too inaccurate or too unreliable, in theoretical chemistry and materials science alike. In this talk we describe the CC-aims interface, the CC4S code, and demonstrate the application of CC and MP2 by investigating the relative stability of boron nitride phases. - This work received support from the European Union's Horizon 2020 research and innovation program under Grant Agreement No. 951786 (The NOMAD CoE).

[1] Q. Sun *et al.*, J. Chem. Phys. 153:024109 (2020)

[2] E. Moerman *et al.* to be published, J. Open Source Software

[3] The FHI-aims web page: <https://fhi-aims.org>

MM 12.8 Tue 12:15 H44

Wannier function perturbation theory: localized representation and interpolation of wavefunction perturbation — ●JAE-MO LIHM and CHEOL-HWAN PARK — Department of Physics, Seoul National University, Seoul, Korea

Wannier functions provide a localized representation of the electronic structure of solids and are thus finds wide application in condensed matter physics. However, the Wannier function method is limited in that it cannot be used to represent the change of the wavefunctions due to perturbations. In this work, we introduce Wannier function perturbation theory (WFPT) [1], which overcomes this limitation by providing a localized representation of wavefunction perturbation which we term "Wannier function perturbation." Among the diverse possible applications of WFPT, we provide three examples. First, we calculate the temperature dependence of the indirect optical absorption spectra of silicon. Our calculation differentiates phonon-absorption and phonon-emission processes and includes the band-gap renormalization without arbitrary temperature-dependent shifts in energy at the same time,

which is beyond reach of existing methods. Second, we develop a theory for calculating the shift spin current without any band-truncation error and apply it to monolayer WTe₂. Third, we apply WFPT to calculate the spin Hall conductivity of the same material, again without any band-truncation error. WFPT will open up a new way for studying the response properties of the electron states in real materials.

[1] J.-M. Lihm and C.-H. Park, Phys. Rev. X, 11, 041053 (2021)

MM 12.9 Tue 12:30 H44

Boosting first-principles molecular dynamics with orbital-free density functional theory — ●LENZ FIEDLER¹, ZHANDOS A. MOLDABEKOV¹, XUECHENG SHAO², KAILI JIANG², TOBIAS DORNHEIM¹, MICHELE PAVANELLO², and ATTILA CANGI¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf / CASUS — ²Rutgers University Newark

Kohn-Sham density functional theory (KS-DFT) is one of the most important simulation methods in materials science and quantum chemistry. Yet, standard DFT codes exhibit scaling behaviors in terms of system size and temperature that prohibit extended dynamical investigations of materials using DFT driven molecular dynamics simulations (MD), especially towards the warm dense matter regime (WDM). We present a practical hybrid approach that combines orbital-free density functional theory (DFT) with Kohn-Sham DFT for speeding up first-principles molecular dynamics simulations. Equilibrated atomic configurations are generated using orbital-free DFT for subsequent Kohn-Sham DFT molecular dynamics. This leads to a massive reduction of the simulation time without any sacrifice in accuracy. We show results across systems of different sizes and temperature, up to the warm dense matter regime. To that end, we use the cosine distance between the time series of radial distribution functions representing the ionic configurations. Likewise, we show that the equilibrated ionic configurations from this hybrid approach significantly enhance the accuracy of machine-learning models that replace Kohn-Sham DFT.

MM 12.10 Tue 12:45 H44

First-principles calculations of plasma frequency in an all-electron full-potential framework — ●MARIA K. POGODAEVA, SERGEY V. LEVCHENKO, and VLADIMIR P. DRACHEV — Moscow, Russia

We present a first-principles methodology to calculate plasma frequency of using density-functional theory in an all-electron full-potential framework implemented in FHI-aims. The results are compared to the results obtained with pseudopotential approaches and experimental data from photo-emission, absorption, and electron energy loss spectra. We test the approach on seven elemental metals: gold, silver, sodium, copper, palladium, platinum, and aluminum. Our results reproduce experimental values for plasma frequency within 0.1-0.3 eV accuracy compared to experiment for all metals except sodium. Calculated plasma frequency for sodium is consistently overestimated by 0.5 eV by VASP and FHI-aims. For other metals except gold FHI-aims and VASP are in a perfect agreement with each other and with experiment. For gold VASP underestimates plasma frequency by 0.6 eV compared to experiment, but FHI-aims calculates the value within 0.2 eV. Overall, the agreement between the two codes and the experiment is good. This validates our all-electron implementation and allows for further applications of the methodology to more complex systems

MM 13: Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 3

Time: Tuesday 10:15–13:00

Location: H45

Topical Talk

MM 13.1 Tue 10:15 H45

Supercompatibility in ceramic micropillars of lanthanum niobate — ●OLIVIA A. GRAEVE and HAMED HOSSEINI-TOUDESHEKI — University of California San Diego, La Jolla, CA, USA

Superelastic materials represent a distinct family of compounds with the ability to manifest reversible deformation in response to an applied stress. Generally, superelastic materials are metallic in nature, and only very few ceramics have been shown to fully or partially display this response. Here, we describe exceptional superelasticity and enhanced reversibility on micropillars of LaNbO₄ ceramic in response to compressive stresses up to 1100 MPa without fracture. The micropillars were prepared by focused ion beam machining from speci-

mens consolidated by spark plasma sintering. The material response to stress is consistent with the theory of supercompatibility (cofactor theory) that has been reported to address the enhanced reversibility and low-hysteresis behavior (i.e., improved superelasticity) of certain shape memory metallic alloys. This makes LaNbO₄ a unique addition to the germane family of smart materials for applications as long-lived actuators impacting the automotive, energy and aerospace sectors, among many other technologically significant fields, especially in extreme conditions (i.e., higher temperatures or pressures) under which ceramics excel compared to metals.

Topical Talk

MM 13.2 Tue 10:45 H45

X-Ray Spectro(micro)scopy as analytics for field assisted de-

position processes — ●DAVID N. MUELLER — Peter Grünberg Institut, Forschungszentrum Jülich

X-Ray absorption spectroscopy (XAS) is element specific, sensitive to the electronic structure around the Fermi level, and provides information about the short-range order in a material, and can be tuned to be surface sensitive. It therefore represents a versatile tool to assess the impact of external fields during synthesis of functional materials on the structure property relations required for optimizing functionalization. Providing spatial resolution on the sub micrometer scale with X-Ray photoemission electron microscopy (XPEEM) additionally allows identification of phase inhomogeneities and their peculiarities with respect to chemistry and structure.

In this presentation, we will use 3d transition metal based oxides of varying complexity to showcase how XAS and XPEEM can give valuable insights into the atomic and electronic structure and how those can be improved towards use in e. g. catalysis by using external fields during synthesis. It will furthermore be discussed how numerical methods such as principal component analysis can help analyzing spectromicroscopic data to unambiguously identify subtle lateral inhomogeneities in the spectroscopic signatures, providing information about phase formation and decomposition processes.

MM 13.3 Tue 11:15 H45

Magnetic Field-assisted Chemical Vapor Deposition of MgFe₂O₄ Films for Photoelectrochemical Water Splitting — HYENKWON LEE¹, ●ZIYAAD TALHA AYTUNA¹, AMAN BHADRAWAJ¹, MICHAEL WILHELM¹, KHAN LE¹, BENJAMIN MAY², DAVID MÜLLER², and SANJAY MATHUR¹ — ¹Greinstraße 6, 50939 Köln — ²Wilhelm-Johnen-Straße, 52438 Jülich

Single-phase magnesium ferrite films (MgFe₂O₄) were grown by magnetic field-assisted chemical vapor deposition (CVD) of mixed-metal precursor [MgFe₂(OtBu)₈] as a function of the applied field strength (B = 0.0, 0.5 and 1.0 T). The formation of monophase MgFe₂O₄ deposits was confirmed by X-ray diffraction and photoelectron spectroscopy. The cross-sectional analysis (FIB-SEM) of the film revealed an increased densification and crystal growth, upon application of the magnetic field when compared to zero-field deposition. The MgFe₂O₄ films deposited under zero-field and field-assisted conditions were used as electrodes in a photoelectrochemical (PEC) water-splitting reaction. All the three samples showed a stable performance and photocurrent values, however, the photocurrent was found to gradually decrease with increasing applied magnetic field (0 T: 5.74 μA/cm², 0.5 T 2.33 μA/cm², and 1 T: 1.33 μA/cm² at 1.23 V (vs. RHE)), which is possibly due to change in absorption properties and crystal orientation, decreasing photo absorption intensity provided by the UV-vis results and the latter being evident in the disappearance of (220) peak in MgFe₂O₄ films grown under the influence of the external magnetic field.

15 min. break

MM 13.4 Tue 11:45 H45

PECVD carbon-coated electrospun vanadium pentoxide nanofibers as cathode material for photoresponsive batteries — ●MICHAEL WILHELM, RUTH ADAM, AMAN BHADRAWAJ, and SANJAY MATHUR — University of Cologne, Cologne, Germany

Harvesting and converting sunlight as the most sustainable energy source on earth is still challenging. Photo-rechargeable batteries represent a synergistic concept that integrates both energy harvesting and energy storage modalities based on dual-functional materials. Vanadium pentoxide nanofibers (VNF) as photoresponsive material was synthesized by electric field-assisted spinning technique and used as dual-action cathode material for photo-rechargeable lithium-ion batteries. A high discharge capacity was delivered, which could be increased under light illumination confirming the photoresponsive behavior. To minimize side reactions and to increase the stability of the electrodes, the VNF were carbon-coated by plasma-enhanced chemical vapor deposition (PECVD). Long-term stability tests showed that besides being a conductive shell, the carbon coating is also essential in retaining the structural instability of VNF. Higher capacity retention upon cycling compared to the non-carbon-coated VNF (after 300 cycles: 43.85 % capacity retention VNF and 61.13 % capacity retention for carbon-coated VNF). Further, the rechargeability of the material by light was demonstrated by illuminating with a UV lamp and after-

ward discharging the electrode material in the dark which delivered a photoconversion efficiency of 4.24 % for VNF and 5.07 % for carbon-coated VNF.

MM 13.5 Tue 12:00 H45

Structure and Morphology Engineering of Hexagonal Boron Nitride (h-BN) using Magnetic Field assisted CVD — ●ANJA SUTORIUS, MICHAEL WILHELM, KHAN LÊ, ZIYAAD AYTUNA, and SANJAY MATHUR — University of Cologne, Cologne, Germany

The aim for two dimensional materials namely graphene, MoS₂ and borophene has become a high interest due to their amazing properties (e.g. conductivity, flexibility, dimensionality) and demand for innovative electronic device applications. The large band gap material h-BN catches the attention of latest research due to its non-toxicity, environmentally friendly and chemical stability as well as its dielectric properties. The commonly preparation of h-BN often requires a gas phase deposition on catalytic metals at very high temperatures and is despite intense research very challenging. A new opportunity is provided using an external magnetic field during synthesis. Precursor molecules like amino borane (NH₃BH₃) or dimethyl amino borane (CH₃)₂NBH₂ and h-BN itself exhibit a charge distribution and thus can be influenced by an applied field. Here, we would like to report about the thin film formation of h-BN with and without an external magnetic field on a variety of substrates ranging from catalytic metal substrates to non-catalytic dielectric silicon substrates. Results from infrared and x-ray photoelectron spectroscopy, as well as transmission and scanning microscopy.

MM 13.6 Tue 12:15 H45

Nanocrystalline CoCrFeNiGax (x = 0.5, 1.0) high entropy alloys: structural and magnetic features — ●NATALIA SHKODICH, MARINA SPASOVA, and MICHAEL FARLE — Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany

Nanocrystalline single fcc phase CoCrFeNiGax (x = 0.5, 1.0) high entropy alloy (HEA) powder particles with good structural and compositional homogeneity were successfully fabricated by high energy ball milling (HEBM). Characterization by XRD, SEM/EDX, and TEM/EDX shows that the fcc phase with the refined microstructure of nanosized grains (~10 nm) could be obtained after 190 min of HEBM at 900 rpm. We used HEBM powders to fabricate homogeneous nanocrystalline bulk HEAs by spark plasma sintering (SPS). SPS at 1073 K of the CoCrFeNiGa_{0.5} HEA powder increases the crystallinity of the fcc phase, while for the equiatomic CoCrFeNiGa powder a partial transformation of the fcc into the bcc phase is observed. The nanocrystalline HEA CoCrFeNiGax (x = 0.5, 1.0) powders show a paramagnetic behavior at room temperature and a Curie temperature (T_c) is of 127K-130K. After SPS, the CoCrFeNiGa bulk material is ferromagnetic up to T_c = 775K. Its saturation magnetization M_s (300K) increases by a factor of 10 as compared to the HEA powder. The SPS of the CoCrFeNiGa_{0.5} HEA powder, however, does not change its paramagnetic nature at ambient temperature. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG) within CRC/TRR 270, project S01 (project ID 405553726).

Topical Talk

MM 13.7 Tue 12:30 H45

Field-assisted processing of magnetic materials — ●FERNANDO MACCARI and OLIVER GUTFLEISCH — Technical University of Darmstadt, 64287 Darmstadt, Germany

Optimization of materials requires a precise control of processing parameters to achieve a desired combination of phases and microstructural features. The application of an external fields during synthesis, going beyond the classical use of only temperature and time, can be used as additional degree of freedom to promote densification, solid state phase transformation, intermetallic compounds and precipitates formation. This combination opens new possibilities to obtain highly tailored microstructures and improved properties.

Focusing on magnetic materials, this talk will provide an overview on how different length scales can be manipulated using external magnetic and electric field assisted processing techniques to create materials with enhanced functional properties. Aspects related to induced magnetic anisotropy and phase formation in soft and hard magnetic materials will be covered. Additionally, field driven coupled magnetic and phase transition is going to be addressed and exemplified in ferromagnetic shape memory Ni-Mn-Ga Heusler compound.

MM 14: Materials for Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 10:15–11:30

Location: H46

MM 14.1 Tue 10:15 H46

How Important are Long-Range Electrostatics in Machine-Learning Potentials for Battery Materials? — ●CARSTEN STAACKE¹, HENDRIK HEENEN¹, CHRISTOPH SCHEURER¹, GABOR CSANYI², KARSTEN REUTER¹, and JOHANNES MARGRAF¹ — ¹Fritz Haber Institut, Berlin, Germany — ²Engineering 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 $\text{Li}_7\text{P}_3\text{S}_{11}$ glass-ceramic have gained much attention. Modern machine learning (ML) potentials are increasingly being adopted as a tool for modeling SSEs at the atomistic level. However, the local nature of these ML potentials typically means that long-range contributions arising, e.g., from electrostatic interactions are neglected. To this end, we have combined short-ranged machine-learning potentials based on the Gaussian Approximation Potential (GAP) approach with a classical electrostatic model in the long-range (ES-GAP). We will present a first-principles validation of both, the pure GAP potential and the new ES-GAP for the LPS SSE. In particular, the role of Coulomb interactions in isotropic vs. non-isotropic system simulations will be evaluated. In standard isotropic simulation tasks, such as determining ionic conductivities, both GAP and ES-GAP yield similar results. In contrast, simulations on non-isotropic systems show the importance of ES contributions and provide new insights into interface stability of $\text{Li}_7\text{P}_3\text{S}_{11}$.

MM 14.2 Tue 10:30 H46

Oxygen Hole Formation Controls Stability in LiNiO_2 Cathodes: DFT Studies of Oxygen Loss and Singlet Oxygen Formation in Li-Ion Batteries — ●ANNALENA GENREITH-SCHRIEVER^{1,3}, HRISHIT BANERJEE^{1,2,3}, CLARE P. GREY^{1,3}, and ANDREW J. MORRIS^{2,3} — ¹Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, United Kingdom — ²School of Metallurgy and Materials, University of Birmingham, Birmingham, United Kingdom — ³The Faraday Institution, Harwell Science and Innovation Campus, Didcot, United Kingdom

Ni-rich cathode materials achieve both high voltages and capacities in Li-ion batteries but are prone to structural instabilities and oxygen loss via the formation of singlet oxygen. Using ab initio molecular dynamics simulations, we observe spontaneous O_2 loss from the (012) surface of delithiated LiNiO_2 , singlet oxygen forming in the process. We find that the origin of the instability lies in the pronounced oxidation of O during delithiation, i.e., O plays a central role in Ni-O redox in LiNiO_2 , as analysed with density-functional theory and dynamical mean-field theory calculations based on maximally localised Wannier functions. The O_2 loss route observed here consists of 2 surface O^- radicals combining to form a peroxide ion, which is oxidised to O_2 , leaving behind 2 O vacancies and 2 O^{2-} ions: effectively 4 O^- radicals disproportionate to O_2 and 2 O^{2-} ions. Singlet oxygen formation is caused by the singlet ground state of the peroxide ion, with spin conservation dictating the preferential release of $^1\text{O}_2$.

MM 14.3 Tue 10:45 H46

Defects and Phase Formation in Non-Stoichiometric LaFeO_3 : A Combined Theoretical and Experimental Study — ●DANIEL MUTTER¹, ROLAND SCHIERHOLZ², DANIEL URBAN¹, SABRINA HEUER^{2,3}, THORSTEN OHLERTH^{2,3}, HANS KUNGL², CHRISTIAN ELSÄSSER^{1,4}, and RÜDIGER-A. EICHEL^{2,3} — ¹Fraunhofer IWM, Freiburg — ²Forschungszentrum Jülich, IEK-9 — ³RWTH Aachen, Institute of Physical Chemistry — ⁴FMF, Universität Freiburg

Defect engineering of perovskite compounds has become increasingly popular as it offers the possibility to influence their catalytic properties for applications in energy storage and conversion devices such as solid-oxide fuel- and electrolyser cells. We present results of a combined theoretical and experimental study exploring the feasibility for an ac-

tive manipulation of the La stoichiometry, and thereby the valence state of Fe, in LaFeO_3 , which can be regarded as a base compound of the family of catalytically active $\text{La}_{1-x}\text{A}_x\text{Fe}_{1-y}\text{B}_y\text{O}_{3-\delta}$ compounds. Concentrations of point defects are presented, derived from formation energies which were calculated by first-principles DFT+U calculations as a function of experimental processing conditions, resulting in predictions of achievable stoichiometry ranges. In the experimental part, LFO was synthesized with a targeted La-site deficiency, and we analyzed the phases in detail by X-ray diffraction and various electron microscopy methods (STEM, EDS, EELS). Instead of a variation of the La/Fe ratio, a mixture of two phases, $\text{Fe}_2\text{O}_3/\text{LaFeO}_3$, was observed, resulting in an invariant charge state of Fe, which is in line with the theoretical results.

MM 14.4 Tue 11:00 H46

Can we improve thermoelectric properties by microstructural manipulations? — ●LEONIE GOMELL¹, TOBIAS HAEGER², MORITZ ROSCHER¹, HANNA BISHARA¹, RALF HEIDERHOFF², THOMAS RIEDL², CHRISTINA SCHEU¹, and BAPTISTE GAULT¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland — ²Institute of Electronic Devices, University of Wuppertal, Deutschland

Thermoelectric (TE) materials convert (waste) heat into electrical energy. Several material properties determine TE performance, with the influence of microstructure being the least understood. However, the microstructure plays a crucial role in the performance of TE materials.

We present microstructural investigations of Fe_2VAl , synthesized via laser surface remelting. Scanning electron microscopy and atom probe tomography were used to bridge the scale from nanometer to micrometer. The local electrical resistivity was analyzed by an in-situ four-probe technique and the thermal conductivity by scanning thermal microscopy.

We observed a high dislocation density in the order of 10^{13} m^{-2} and small grains separated by low-angle grain boundaries. Segregation of V and N was found at grain boundaries and dislocations, observed by atom probe tomography. These defects scatter electrons and phonons, influencing their transport within the material.

We conclude that by manipulating the microstructure, we were able to improve the properties of Fe_2VAl . The combination of detailed microstructural analysis and local measurement of properties offers the possibility of understanding the microstructure-property relationship.

MM 14.5 Tue 11:15 H46

Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation — ●JIAJIA QIU^{1,2}, HUAPING ZHAO¹, WENHUI MA², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Recently, a growing interest of incorporating graphene (Gr) with silicon (Si) to develop Gr-Si Schottky junction solar cells is considered as a potential low-cost alternative to the conventional p-n junction silicon solar cells. In this work, silicon nanowires (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of Gr-Si solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs/SiIPs solar cell were systematically analyzed. The results show that the inverted pyramid arrays have ability of balance of antireflectance and surface area simultaneously. Compared to the Gr-SiNWs solar cells, power conversion efficiency (PEC) and carrier lifetime of Gr-SiIPs devices increase by 62% and 34%, respectively. Finally, the Gr-SiIPs cell with efficiency of 5.63% was successfully achieved through doping nitric acid. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

MM 15: Hydrogen in Materials: Hydrogen Effects

Time: Tuesday 11:45–13:00

Location: H46

MM 15.1 Tue 11:45 H46

Atomistic study of hydrogen behavior in bcc and fcc Fe in presence of crystal defects — ●DARIA SMIRNOVA¹, SERGEI STARIKOV², TAPASWANI PRADHAN², RALF DRAUTZ², and MATOUS MROVEC² — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Ruhr University Bochum, ICAMS, Bochum, Germany

We apply atomistic simulations to consider hydrogen behavior in Fe in presence of the given lattice distortions, namely, crystal defects or lattice expansion/compression due to applied stresses. Simulations are based on a new interatomic potential developed by the authors of current work. Firstly, we consider segregation of hydrogen on typical defects of different complexity: from vacancies to grain boundaries (GBs). Estimated segregation energies obtained for different types of GBs generally agree with the existing DFT data. Moreover, performed classical atomistic simulations give information on several types of GBs, which, due to their complex structure and considerable model size, are inaccessible for ab initio modeling. High-temperature simulations of H diffusion in the presence of GBs also show that for bcc Fe hydrogen diffusion coefficient in the GB is much lower than in bulk. The same type of study is carried out for fcc Fe. Also, we discuss variations in zero-temperature hydrogen migration barriers in bulk bcc Fe with applied stress and compare them with the results of the finite-temperature H diffusion simulations. We see that while the variations in the lattice parameter change hydrogen migration barrier, they give no significant impact on the finite-temperature hydrogen diffusion.

MM 15.2 Tue 12:00 H46

Interplay of hydrogen with defects in Al alloys — ●POULAMI CHAKRABORTY¹, HUAN ZHAO¹, BAPTISTE GAULT^{1,2}, TILMANN HICKEL^{1,3}, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — ²Department of Materials, Royal School of Mines, Imperial College London, United Kingdom — ³BAM Federal Institute for Materials Research and Testing, Berlin, Germany

Al alloys are used as major structural material in the aviation and more recently, automobile industries. This demands detail research of microstructural defects generated while usage. We have performed density functional theory calculations to study the competition of microstructural features including grain boundaries and second phase particles. The results reveal second phases as better trapping sites since H has a higher solubility compared to the GBs. However, it is seen that certain solutes such as Mg enhances the chance of HE at the forming surface during crack initiation. This is further supported by experimental data where a high strength 7xxx Al alloy is charged by deuterium using atom probe tomography (APT). Subsequently, we have extended our study to several other alloying elements such as Sc, Sn and Zr, at the GB which are inevitably present as impurities in technical alloys. Interestingly, it is seen that Sn strongly binds with H at the GB without increasing the embrittling tendency. Based on these insights, effective alloying strategies can be developed to improve the resistance to hydrogen embrittlement.

MM 15.3 Tue 12:15 H46

Impact of H on Fe and Cr diffusion in pure Fe and FeCr alloy — ●OLGA LUKIANOVA¹, ANTON CHYRKIN², VLADISLAV KULITCKII¹, JAN FROITZHEIM², SERGEI STARIKOV³, GERHARD WILDE¹, RALF DRAUTZ³, and SERGIY DIVINSKI¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Chalmers University of Technology, Department of Chemistry and Chemical Engineering, Division of Energy and Materials, Gothenburg, Sweden — ³ICAMS,

Ruhr-Universität Bochum, Bochum, Germany

The impact of hydrogen on the tracer diffusion of the Fe and Cr in pure iron and Fe-18wt.%Cr alloy was measured at 873 K. The annealing treatments were performed in purified argon (H-free) and Ar+H₂ atmospheres. Volume diffusion of Cr was found not to be affected by the presence of H in both alpha-Fe and the FeCr alloy whereas volume diffusion of Fe was enhanced by an order of magnitude. On the contrary, grain boundary diffusion of Cr in the FeCr alloy was retarded, while it was not affected by hydrogen in pure iron. Grain boundary diffusion of Fe remains practically unchanged in both materials. The tracer data are compared with the predictions from atomistic simulations.

MM 15.4 Tue 12:30 H46

Correlation of hydrogen diffusion behavior and in situ micro-mechanics during hydrogen charging of bcc Fe-Cr alloys — ●MARIA JAZMIN DUARTE CORREA, JING RAO, and GERHARD DEHM — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Hydrogen (H) is a strong candidate as energy carrier but it might cause material degradation through hydrogen embrittlement. Individual hydrogen-microstructure interactions, can be studied by targeting analyses at the nano-/microscale during H exposure. We will present our novel *back-side* electrochemical H charging approach for nanoindentation related techniques. Hydrogen diffusion from the charged back-side towards the testing (front) surface is quantified by Kelvin probe permeation tests and unwanted corrosion is avoided. Our unique method allows differentiating between the effects of trapped and mobile H, and performing well controlled measurements with different H levels monitored over time to consider H absorption, diffusion and release through the metal. These aspects will be presented by nanoindentation and micropillar compression tests during H charging of Fe-Cr alloys (8-20 wt.%Cr). An enhanced dislocation nucleation is shown consistent with the defactant theory, and a hardening effect while increasing the Cr content and the H entry. The mechanical data is finally analyzed in terms of the diffusion behavior and used to develop a nanohardness-based H diffusion coefficient approach.

MM 15.5 Tue 12:45 H46

Role of hydrogen on the relative stability of the phases in steels — ●ALI TEHRANCHI, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max Planck institute for Iron research, Max Planck Straße 1, 40237 Düsseldorf

Hydrogen embrittlement (HE) is a persistent mode of failure in high-strength steels. During the service life of these steels phase transformations occur and are a key element that determines their response to the service loads. Thus the investigation of the role of H atoms in the relative stability of the phases present and forming in steels is of great interest. In this work, we studied the role of H on the relative stability of the fcc/bcc/hcp phases using the ab initio thermodynamics. The results indicate that at low hydrogen chemical potentials the stability of the fcc phase, which can be representative of retained austenite (RA) in steels, is slightly enhanced by the presence of H atoms. In contrast, at high hydrogen chemical potentials the bcc phase is stabilized by H. Moreover, since the excess volume of the hydrogen-rich bcc phase is significantly larger than that of the fcc phase, the presence of a stress field can change the relative stability of these phases in the coexistence regions of the phase diagram. This feature is particularly important for cyclic loading conditions: during loading cycles forward and reverse phase transformations occur and the H released by these transformations can damage the material.

MM 16: Mechanical Properties

Time: Tuesday 14:00–15:00

Location: H44

MM 16.1 Tue 14:00 H44
co-electrodeposition of compositionally complex co-cr-fe-mo-ni alloy thin films — ●HONGSHUAI LI, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Co-Cr-Fe-Mo-Ni, a compositionally complex alloy with a face-centered cubic structure, was successfully obtained by electrochemical deposition. To achieve a smooth morphology, an aqueous electrolyte with several additives was used as the solution for electrodeposition. Since the characterization of the sample requires a certain thickness, the electrodeposition time was set to 10 min. Characterization of the film deposited under a constant current density reveals the deposit is metallic with a face-centered cubic structure. The adhesion properties as well as the effective mechanical performance have also been tested by nano-scratch experiments, indicating a microscopically ductile behavior. The electrolytes developed in this study may be a promising approach for the electrodeposition of Co-Cr-Fe-Mo-Ni medium entropy alloys.

MM 16.2 Tue 14:15 H44
orientation dependence of the deformation mechanisms of cocrfeni high entropy alloys — ●HAIHONG JIANG, MARTIN PETERLECHNER, and GERHARD WILDE — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

The mechanical behavior of CoCrFeNi high entropy alloys in different deformation states have been analyzed by nanoindentation. Microhardness and Young's modulus values were determined at high accuracy as a function of the specified crystallographic orientations, which were measured by electron backscatter diffraction (EBSD). Modulus and Poisson's ratio values of polycrystalline CoCrFeNi were calculated from experimentally determined ultrasonic velocities for comparison. This approach allows for in-depth analysis and comparison of the mechanical properties as function of the local orientations of the crystal lattice in dependence of the thermo-mechanical history.

MM 16.3 Tue 14:30 H44
Influence of crack tip radius on fracture toughness: an atomistic study — ●TARAKESHWAR LAKSHMIPATHY¹ and ERIK BITZEK^{1,2} — ¹Department of Materials Science and Engineering, In-

stitute I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany — ²Department Computational Materials Design, Max-Planck-Institut für Eisenforschung, Germany

In fracture mechanics, initial cracks are typically assumed to be infinitely sharp, leading to a singularity in the crack tip stress field. However, on the atomic scale, crack tips have a radius of at least one atomic distance, which removes the singularity and leads to high, but finite stresses directly at the crack tip. Furthermore, cracks may blunt due to various reasons which leads to an increase in the macroscopic stress to reinitiate a sharp crack. Using harmonic "snapping spring" nearest-neighbor potentials which provide the closest match to linear elastic fracture mechanics (LEFM) on a discrete lattice, we show that the LEFM model for sharp cracks is insufficient to describe the boundary value problem (BVP) of blunted cracks at the atomic scale. We also show that the LEFM-based equations for blunted cracks are insufficient to describe the stress distribution ahead of atomically blunted cracks. We develop a semi-empirical scaling relation for blunted cracks using the LEFM-based equations for elliptical cracks by introducing a factor to account for the deviations. Furthermore, we identify a lower bound for the maximum crack tip radius at which this factor stops playing a role and a scaling model from the unmodified LEFM-based equations for elliptical cracks can be used.

MM 16.4 Tue 14:45 H44
Interplay of Cottrell atmosphere formation and carbon ordering in ferrite — ●SAM WASEDA, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Dusseldorf, Germany

In common steels, carbon atoms are purportedly or unintentionally added and alter mechanical properties of the steels. In ferrite, it is proposed that much of them does not stay as solid solution and ends up in the following possibilities: 1, segregate to structural defects; 2, make an elastically favorable ordered structure (Zener-ordering); 3, diffuse to other phases or form a precipitate (austenite, cementite etc.). While they are individually well studied, the interplay between these different scenarios is hardly studied. In this work, we present a density-based diffusion model to study the chemical and elastic interactions between Fe and C as well as among C, in order to understand the interplay between the formation of Cottrell atmospheres and the Zener-ordering.

MM 17: Hydrogen in Materials: Hydrogen Storage

Time: Tuesday 14:00–15:15

Location: H46

MM 17.1 Tue 14:00 H46
Open system mechanical behavior of nanoporous palladium-platinum-hydrogen solid solution near critical point — ●SAMBIT BAPARI and JÖRG WEISSMÜLLER — Werkstoffphysik und technologie, Technische Universität Hamburg

Bulk nanoporous palladium is an ideal system for studying open system elasticity as palladium with randomly oriented nanometer size ligaments affords rapid equilibration of hydrogen between an environment and the materials bulk [1]. In this work, nanoporous palladium-platinum (5 at%) alloy was prepared by electrochemical dealloying. Transmission electron microscopy, oxygen adsorption*desorption methods were used to characterize the morphology and structure of the nanoporous alloy. The average ligament size of the as dealloyed nanoporous palladium-platinum alloy is 4 nm compared to 20 nm for nanoporous palladium. Hydrogen solubility isotherms show near critical point behavior in palladium-platinum-hydrogen solid solution at room temperature. Solute susceptibility and concentration-strain coefficient were determined to estimate the difference in compliance between open and closed systems. In situ quasistatic mechanical tests and strain rate jump tests were conducted to analyze the open system elastic and plastic deformations at near critical point. [1] S Shi, J Markmann, J Weissmüller. Verifying Larché-Cahn elasticity, a milestone of 20th-century thermodynamics, PNAS, 2018,115 (43) 10914-10919

MM 17.2 Tue 14:15 H46
Metal-organic frameworks for hydrogen isotope separation — ●MICHAEL HIRSCHER — Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

One of the important operations in chemical industry is separation and purification of gaseous products. Especially H₂/D₂ isotope separation is a difficult task since its size, shape and thermodynamic properties resemble each other. Porous materials offer two different mechanisms for separating hydrogen isotopes, either confinement in small pores, i.e., *kinetic quantum sieving*, or adsorption on strong binding sites, i.e., *chemical affinity quantum sieving*. The new class of metal-organic frameworks (MOFs) allows the exact tailoring of pore size and aperture as well as including open metal sites into the framework. Furthermore, if MOFs consist not of a static, but flexible framework, they can reversibly respond to external stimuli, which may even enhance the separation selectivity.

Experimentally, the measurement of the selectivity for hydrogen isotope separation is very challenging, since it requires low temperatures near the boiling point of the gases. Using low-temperature thermal desorption spectroscopy (TDS), we have developed a method for measuring directly the isotope selectivity after exposure to H₂/D₂ mixtures.

Exemplarily, this talk will present experimental results on hydrogen isotope separation in MOFs.

MM 17.3 Tue 14:30 H46

Microstructural study of MgB₂ in the LiBH₄-MgH₂ composite by TEM — ●OU JIN¹, YUANYUAN SHANG², XIAOHUI HUANG¹, XIAOKE MU¹, DOROTHÉE VINGA SZABÓ¹, THI THU LE², STEFAN WAGNER¹, CHRISTIAN KÜBEL³, CLAUDIO PISTIDDA², and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology, Karlsruhe, Germany — ²Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — ³Technical University of Darmstadt, Darmstadt, Germany

The LiBH₄-MgH₂ composite is known as Reactive Hydride Composite for hydrogen storage that has an exceptional hydrogen storage capacity (up to ~ 12 wt% H₂) and enhanced thermodynamic properties (down to ~ 45 kJ/mol H₂). The main challenge that limits the extensive application of this material is its sluggish kinetic performance, which is primarily ascribed to the hampered nucleation of MgB₂ during decomposition. It was found that transition metal-based additives could facilitate the formation of MgB₂ and accelerate the decomposition of LiBH₄-MgH₂. However, the additive effect on the kinetic improvement had not been fully understood until now. To unravel the uncertainties, the formation of MgB₂ in the decomposed LiBH₄-MgH₂ with and without the additive 3TiCl₃-AlCl₃ was studied using manifold transmission electron microscopy techniques. Varied MgB₂ morphologies have been determined, originating from different nucleation centers. Given the heterogeneous nucleation, the crystallographic orientation relationship of the relevant phases is in depth discussed. It turns out that atomic misfit plays a dominant role and directly affects the in-plane strain energy density, leading to varied kinetic performance.

MM 17.4 Tue 14:45 H46

ETEM studies on hydride precipitation and growth in Mg films — MAGNUS HAMM¹, MARIAN DAVID BONGERS¹, VLADIMIR RODATIS¹, STEFAN DIETRICH², KARL-HEINZ LANG², and ●ASTRID PUNDT² — ¹Göttingen University, Institute of Materials Physics (IMP), Göttingen, Germany — ²Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Materials Science and Engineering (IAM-WK), 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 17.5 Tue 15:00 H46

Recycling as the key for developing sustainable hydrogen storage materials — ●CLAUDIO PISTIDDA¹, YUANYUAN SHANG¹, THI THU LE¹, GOKHAN GIZER¹, HUJUN CAO¹, NILS BERGEMANN¹, RIFAN HARDIAN¹, MARTIN DORNHEIM¹, and THOMAS KLASSEN^{1,2} — ¹Department of Materials Design, Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany — ²Helmut Schmidt University, Holstenhofweg 85, 22043, Hamburg, Germany

Metals play a crucial role in supporting the global economy and the wellbeing of humankind. Supported by the constantly increasing demand for metal-based products, the extraction of mineral resources has increased, over the last decades, at a faster rate than economic growth. This trend is forecasted to steadily increase in the near future, thus leading to concerns over the exploitation of the Earth's natural resources and the environmental impact that the extraction of metals will have. In this scenario, finding new ways to recycle metals and metal alloys, even those of low purity, is mandatory.

To reduce the carbon footprint and environmental impact that the mining of metals for hydrogen storage purposes entails and to reduce their cost, at the Helmholtz-Zentrum Hereon we pursue the possibility of obtaining high-quality hydride-based materials from industrial metal waste. A complete overview of recent scientific breakthroughs in the synthesis and characterization of hydrogen storage materials made from recovered metal wastes will be presented.

MM 18: Poster Session 2

Time: Tuesday 17:30–20:00

Location: P2

MM 18.1 Tue 17:30 P2

Thermal transport properties of sodium superionic conductors from molecular dynamics simulations — ●INSA DE VRIES, FREYA HALLFARTH, HELENA OSTHUES, and NIKOS DOLTSINIS — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany

Improvements of energy storage systems include the usage of sustainable and low-cost materials. In the case of electrolytes for solid state batteries, this is true for sodium superionic conductors due to the high availability of sodium especially compared to lithium based systems. A proper and safe integration of the electrolyte into battery cells also requires taking into account its thermal properties. Due to the ionic motion enabled by the open crystal structure of the electrolyte, in addition to electronic and phononic parts, a diffusive part also contributes to thermal transport. It is thus important to determine activation barriers for ionic motion and diffusion mechanisms, as they affect the thermal properties.

Equilibrium atomistic molecular dynamics simulations were performed of NaZr₂P₃O₁₂ and Na₃Zr₂Si₂PO₁₂ using a pair potential by Kumar and Yashonath [1]. Besides identifying ionic diffusion pathways, diffusion constants and thermal transport properties were calculated for various temperatures and compared to results from first principles molecular dynamics.

[1] P. P. Kumar and S. Yashonath, J. Am. Chem. Soc. **124**, 3828 (2002)

MM 18.2 Tue 17:30 P2

hiphive - Constructing and sampling higher order force constants for strongly anharmonic materials — ●ERIK FRANSSON¹, FREDRIK ERIKSSON¹, JOAKIM BRORSSON¹, ZHEYONG FAN², and PAUL ERHART¹ — ¹Chalmers University of Technology, Gothenburg, Sweden — ²Aalto, University Helsinki Finland

Higher order force constants (FCs) play a key role in lattice dynamics and are crucial for the analysis of many thermodynamic material properties. Typically FCs have been extracted using the finite displacement method, which suffers, however, from poor scaling with order and system size. In this contribution we present updates to and applications of the python package hiphive, a tool that allows the efficient extraction of FCs via a regression approach, both up to high order and for low symmetry systems. Higher order FCs can be used to directly run molecular dynamics (MD) simulations, however for strong anharmonic materials these models can become unstable. To overcome this obstacle, we present a self-consistent (iterative) approach for training higher order FCs and demonstrate its effectiveness for multiple strongly anharmonic materials. We have furthermore interfaced hiphive with the GPUMD software, which enables large scale molecular dynamics simulations using FC expansion potentials. This allows for sampling of, e.g., thermal conductivity via Green-Kubo techniques. This approach of extracting higher order FCs and sampling thermal conductivity is demonstrated for two very anharmonic materials, SnSe and BaGaGe. Lastly, we also demonstrate the application of this approach to study the complex dynamics of inorganic halide perovskites.

MM 18.3 Tue 17:30 P2

High-throughput calculations for property maps of solids — ●DANIELA IVANOVA¹, DANIEL WORTMANN¹, STEFAN BLÜGEL¹, and MATTHIAS WUTTIG² — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — ²Department of Physics, RWTH Aachen University, Aachen, Germany

Over the last two decades, high-throughput computation has become a vital pillar of the scientific research and development process in the field of computational science. In order to forecast material properties for a larger sets of atomic configurations, Density Functional Theory (DFT) as a widely utilized and high-predictive-power first-principles

approach, has become increasingly frequent to be used robust and automated. In this work, the DFT open-source of an integrated suite of codes for electronic-structure calculations, Quantum ESPRESSO is used as connected and deployed through the open source Automated Interactive Infrastructure and Database for Computational Science AiDA framework to achieve automation. Aside from the existence of (1) covalent, (2) metallic, and (3) ionic bonding, as well as the two weaker forms of (4) hydrogen and (5) van der Waals bonding, compelling evidence has been found that a new bonding mechanism prevails in crystalline phase change materials, termed as*(6)'metavalend bonding*. The materials data set chosen for high-throughput computing and calculation of the relevant materials properties supplies essential data for mapping distinctions between the bonding mechanisms. Such property maps can also lead to the conjecture of a sixth bonding mechanism (MVB).

MM 18.4 Tue 17:30 P2

High Performance Computing as enabler for condensed matter research — ●ANDREAS STRAUCH, JENS FÖRSTNER, THOMAS KÜHNE, and CHRISTIAN PLESSL — Paderborn University, Paderborn, Germany

The availability of High Performance Computing resources has enabled a wide range of high-impact science in the field of condensed matter physics in the last decades. We review the numerical research performed at the Paderborn Center for Parallel Computing (PC²) ranging from atomistic ab-initio-calculations to electromagnetic, optoelectronic, and quantum dynamical simulations. Combining in-depth knowledge on high performance computing and on heterogeneous hardware architectures with topical research has led to the development of high-level hardware-agnostic parallel-computing frameworks like HighPerMeshes [1] and to research on novel numerical methods, e.g. for molecular dynamics simulations [2,3].

[1] S. Alhaddad et al, "The HighPerMeshes framework for numerical algorithms on unstructured grids", *Concurrency and Computation: Practice and Experience* (2021), pp. e6616, DOI: 10.1002/cpe.6616 (2022)

[2] R. Schade et al, "Towards electronic structure-based ab-initio molecular dynamics simulations with hundreds of millions of atoms", *Parallel Computing* 111, doi:10.1016/j.parco.2022.102920 (2022)

[3] R. Schade et al, "Breaking the Exascale Barrier for the Electronic Structure Problem in Ab-Initio Molecular Dynamics", arXiv:2205.12182 (2022)

MM 18.5 Tue 17:30 P2

Computational studies of liquid chromophores — ●ERIC LINDGREN — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Liquid chromophores such as perylene and its derivatives constitute an important class of materials, with applications ranging as solvent-free dyes to increasing the efficiency of solar cells via photon conversion. Their structural and in particular dynamical behaviour on the molecular level is not very well known, yet crucial for their optical properties. In this work, we use molecular dynamics (MD) simulations to investigate the structural and dynamical properties of perylene and two of its derivatives (perylene-ethyl and perylene-diimide). Specifically, we extract the static and dynamical structure factors and the current correlation functions for various temperatures as well as for two different initial structural models of the systems, which in principle allows us to establish a direct link to experimental studies. Motivated by recent experimental work by Hultmark et al. (*Science Advances* 7.29 (July 2021)), we consider two structural models that differ with respect to the relative orientation of the molecules. Whereas in model 1 the molecules are more or less randomly oriented, model 2 features domains with pronounced pi-pi stacking. The latter configuration corresponds to a simplified representation of the supramolecular aggregates that some extended perylene derivatives have been observed to form experimentally. At the moment we have established our simulation protocol and verified the basic premise of this project. Next we will extend our study to derivatives with larger sidegroups and mixtures thereof.

MM 18.6 Tue 17:30 P2

Edge states in proximitized graphene ribbons and flakes in a perpendicular magnetic field: Emergence of lone pseudohelical pairs and pure spin-current states — ●YAROSLAV ZHUMAGULOV, TOBIAS FRANK, and JAROSLAV FABIAN — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany
Graphene influenced by the valley-Zeeman intrinsic spin-orbit coupling through proximity effects provides signatures of pseudohelical edge

states. Analyzing the band structure of a zigzag graphene nanoribbon in the presence of proximity induced spin-orbit interaction and an external magnetic field, we have discovered the effect of stabilization of intervalley edge states and removal intravalley edge states by the external magnetic field. Stabilization of states is associated with the closing/reopening of the bulk bandgap between nonzero Landau levels. The magnitude of the external magnetic stabilization field was estimated both numerically and analytically. Finally, we have found that stabilized intervalley edge states in the presence or in the absence of a spin-flip hopping through the armchair edge form pseudohelical states or pure spin current states, respectively. The states of pure spin current are formed in wide graphene flakes and are protected from scattering by defects on the zigzag edges of graphene flakes. This work was supported by DFG SPP 2244, DFG SFB 1277 and EU Graphene Flagship.

MM 18.7 Tue 17:30 P2

Modelling mechanical bond scission of amine cured Epoxy resins under stress — ●SAMPANNAI PAHI¹, MATTIA LIVRAGHI¹, CHRISTIAN WICK^{1,2}, and ANA-SUNCANA SMITH^{1,3} — ¹PULS Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — ²Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany — ³Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bos01e9ovi0107 Institute, 10000 Zagreb, Croatia

Epoxy resins are widely used thermoset polymers in manufacturing processes. Understanding of fracture propagation in cured epoxy resins is pivotal in determining the bulk level properties of the material. In this paper, a scale-bridging approach that links atomistic molecular dynamics (MD) simulations with DFT based Quantum Mechanical (QM) criterions has been implemented to model bond breakage in Quantum level. In our approach, we create smaller model systems for each bond and implement COGEF procedure to determine optimal bond breakage criterion. Furthermore, a hybrid on-the-fly QM/MM method is described and its ability to capture bond scission on cross linked polymer system with no predetermined fracture site is demonstrated. Using QM bond breakage criterion, bond scission in MD run is identified and checked using presence of spin contamination. Our study provides insights into the molecular mechanisms governing the fracture mechanism of epoxy resins and demonstrates the success of utilising atomistic molecular simulations towards predicting bulk properties.

MM 18.8 Tue 17:30 P2

Solvation effects on proton irradiation of DNA — ●DANIEL MUÑOZ-SANTIBURCIO¹, BIN GU², and JORGE KOHANOFF¹ — ¹Instituto de Fusión Nuclear "Guillermo Velarde", Universidad Politécnica de Madrid, Spain — ²Department of Physics, Nanjing University of Information Science and Technology, China

Proton irradiation of DNA is of utmost importance for many fields, from radiation damage in space to medical applications for cancer treatment. Ab initio simulations are highly valuable tools for understanding such process, but they are cumbersome due to the required level of theory. These involve simulating the non-adiabatic propagation of the electronic subsystem of the target material, and to date have been restricted to DNA systems in absence of water, or at most with few solvating molecules. Here we present the results of large-scale ab initio (RT-TDDFT) simulations of proton irradiation of a realistic DNA system in bulk water, where we have determined different important aspects of the proton irradiation process such as the stopping power of the system, the spacial distribution of the holes in terms of the depopulations of the maximally localized Wannier functions, and more importantly the influence of the surrounding water. We will show that water is neither a mere spectator on the process nor a simplistic reducing or enhancing agent of the excitation process. Instead, water qualitatively changes the excitation landscape of the proton-irradiated DNA, making the hole population on the different atoms and bonds qualitatively different in the solvated vs. the dry DNA case.

MM 18.9 Tue 17:30 P2

Resistometric determination of GP-zone formation and growth — ●FABIAN MILLER, JOHANNES BERLIN, TOBIAS STEGMÜLLER, and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, 86135 Augsburg, Deutschland

Aluminium alloys are of crucial importance in today's economy, therefore the deeper understanding of their mechanical and electrical properties is important. These properties can be influenced by precipitate

formation. In this work we focused in the Al*Cu system with samples containing around 4 wt.% of Cu. They were homogenized at the eutectic temperature and rapidly quenched to ambient temperature. Afterwards 4-point-resistance measurements were conducted during natural and artificial aging. Due to formation of Guinier Preston zones, the resistivity first increases, then slowly decreases, allowing to monitor the unmixing for different temperatures and for different quenching conditions. Further experiments with other alloying metals than Cu will be conducted and variations of the homogenisation temperature are planned to be inspected.

MM 18.10 Tue 17:30 P2

Dealloying and nanoscale structure formation at crystal-melt coexistence — ●ZHONGYANG LI¹, NINA PETERSEN¹, LUKAS LÜHRS¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology — ²Institute of Materials Mechanics, Hybrid Materials Systems, Helmholtz-Zentrum Hereon

Recent work on Ti-Ag alloy has shown that a bicontinuous microstructure can be formed via peritectic melting, which could further transform to open porous Ti or Ag networks through selective etching. Several factors including the large solubility difference of two alloy elements in liquid phase, large composition difference and the volume fraction of the solid and liquid phases are considered to be criteria for this phenomenon. However, the formation mechanism of this particular microstructure during peritectic dealloying is still not fully known.

In this work, alloy systems including Bi-Ni, Fe-Sn and Mn-Sn, are chosen, which satisfy part or all of the aforementioned criteria. With SEM and diffraction experiments of these samples after peritectic melting, we investigate the morphology of different phases, and discuss the dominant factor for the formation of bicontinuous structure. The effect of parameters for thermal treatment, including temperature and duration of heat treatment, are also studied using SEM, in order to find the optimized combination that could produce finer microstructure. With the research in these two aspects, we discuss the possibility of broadening the application of this new dealloying method from peritectic dealloying to dealloying at liquid-solid coexistence state.

MM 18.11 Tue 17:30 P2

Structural and Textural Transitions of Discotic Ionic Liquid Crystals in Nanoporous Solids — ●ZHUOQING LI¹, PATRICK HUBER¹, SABINE LASCHAT², AILEEN RAAB², ANDREAS SCHÖNHALS³, and MOHAMED A. KOLMANGADI³ — ¹Institute for Materials and X-Ray Physics, Technische Universität Hamburg, Hamburg, Germany — ²Institut für Organische Chemie, Universität Stuttgart, Stuttgart, Germany — ³Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Discotic ionic liquid crystals (DILCs) derived from 3,4-dihydroxyphenylalanine (DOPA) have synergetic properties of liquid crystals and ionic liquids. Driven by the $\pi^*\pi$ interactions among the aromatic cores, DILCs may self-organize, leading to a hexagonal ordered columnar liquid crystalline mesophase. Embedding of DILCs in nanoporous solids allows one to design hybrid materials with 1-D ionic conductivity pathways on the single-nanopore scale and tailorable photonic properties. The structural organization of confined DILCs is determined by an interplay of geometrical constraints and interfacial interactions at the pore wall and thus depends on pore size, temperature treatment and molecular wall anchoring. The optical birefringence experiments and small angle X-ray scattering results indicate ordered liquid crystalline mesophases of different collective orientations as a function of anchoring of the DILC discs at the pore surface. In particular, these experiments suggest that depending on the pore size a transition from the formation of circular concentric ring structures to an arrangement, where the columns are aligned parallel to the pore axis occurs.

MM 18.12 Tue 17:30 P2

Laughlin topology on fractal lattices without area law entanglement — ●MANI CHANDRA JHA — MPI-PKS

Laughlin states have recently been constructed on fractal lattices, and the charge and braiding statistics of the quasiholes were used to confirm that these states have Laughlin type topology. Here, we investigate density, correlation, and entanglement properties of the states on a fractal lattice derived from a Sierpinski triangle with the purpose of identifying similarities and differences compared to two-dimensional systems and with the purpose of investigating whether various probes of topology work for fractal lattices. Similarly to two-dimensional systems, we find that the connected particle-particle correlation function decays roughly exponentially with the distance between the lattice sites

measured in the two-dimensional plane, but the values also depend on the local environment. Contrary to two-dimensional systems, we find that the entanglement entropy does not follow the area law if one defines the area to be the number of nearest neighbor bonds that cross the edge of the selected subsystem. Considering bipartitions with two bonds crossing the edge, we find a close to logarithmic scaling of the entanglement entropy with the number of sites in the subsystem. This also means that the topological entanglement entropy cannot be extracted using the Kitaev-Preskill or the Levin-Wen methods. Studying the entanglement spectrum for different bipartitions, we find that the number of states below the entanglement gap is robust and the same as for Laughlin states on two-dimensional lattices.

MM 18.13 Tue 17:30 P2

A study of the local fields in bismuth ferrite by using different radioactive tracer ions — ●THANH T. DANG¹, JULIANA SCHELL^{1,2}, MARIANELA E-CASTILLO¹, DANIL LEWIN¹, ASTITA DUBEY¹, ANDREA G. BOA^{2,3}, REINHARD BECK⁴, CORNELIA NOLL⁴, JOÃO N. GONÇALVES⁵, DMITRY ZYABKIN⁶, KONSTANTIN GLUKHOV⁷, IAN C. J. YAP⁸, ADELEH M. GERAMI^{2,9}, KOEN V. STIPHOUT¹⁰, GEORG MARSCHICK¹¹, EDGAR M. S. D. REIS^{1,2}, SOBHAN M. FATHABAD¹, and DORU C. LUPASCU¹ — ¹University of Duisburg-Essen — ²European Organization for Nuclear Research — ³Technical University of Denmark — ⁴University of Bonn — ⁵Universidade de Aveiro — ⁶TU Ilmenau — ⁷Uzhhorod National University — ⁸Universität Göttingen — ⁹School of Particles and Accelerators — ¹⁰Georg-August-Universität Göttingen — ¹¹Vienna University of Technology

This work presents the study of the local electric and magnetic fields in multiferroic bismuth ferrite using Time Differential Perturbed Angular Correlation spectroscopy. The measurements were carried out at a wide range of temperatures up to 850°C, after the implantation of various radioactive tracer ions: 181Hf, 111In and 111mCd. The experimental results reflect the obedience to Landau theory and Brillouin-Weiss equation of local electric polarization and magnetization, respectively. Particularly, a huge coupling between local electric and magnetic fields has been investigated in anti-ferromagnetic order. With the support of ab-initio DFT simulations, we can conclude that 111mCd is located at Bi-atom, 181Hf and 111In substitute Fe-atom.

MM 18.14 Tue 17:30 P2

Partitioning of transition metals to the γ and γ' phase of Co-based superalloys — ●ISABEL PIETKA¹, ANDREAS FÖRNER², MANUEL KÖBRICH², STEFFEN NEUMEIER², RALF DRAUTZ¹, and THOMAS HAMMERSCHMIDT¹ — ¹Ruhr-Universität Bochum, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science & Engineering

Single-crystal Co-base superalloys are a promising class of materials in high-pressure high-temperature applications such as blades of gas turbines or jet engines. The superior mechanical properties at high temperatures are a consequence of the underlying γ/γ' microstructure. The improvement of the mechanical properties of these alloys is therefore closely tied to an understanding of the influence of alloying elements on the microstructure. In this work, we describe the γ/γ' partitioning of different alloying elements, i.e. their preference for the γ matrix or the γ' particles of the microstructure. In particular, we determine the energy difference of nearly all 3d, 4d, 5d transition metals (TMs) in $\text{Co}_3(\text{Al}/\text{W})$ by density functional theory calculations. In very good agreement with results from wavelength-dispersive X-ray spectroscopy and atom probe tomography, we find a preference of early TMs for the γ' phase while mid to late TMs show no clear preference. We demonstrate that the findings can be rationalized in terms of band-filling and atomic size differences by moment analysis from bond order potential theory.

MM 18.15 Tue 17:30 P2

The oxidation of TNM alloy at 700°C and 760°C — ●HENG ZHANG^{1,2} and YONGFENG LIANG² — ¹Institute of Materials Physics, University of Münster, Germany — ²State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing, China

The TNM sample morphology and components of the oxides are measured with SEM, EDS and XPS after oxidation until 200 hours at 700°C and 760°C respectively. Al_2O_3 is the main oxides at 700°C combined with a little TiO_2 , MoO_2 and MoO_3 , while the oxides are TiO_2 , MoO_2 and MoO_3 at 760°C, exhibiting a good oxidation resis-

tance under 700°C.

MM 18.16 Tue 17:30 P2

Reactive Surface Corrosion of Stainless Steel studied with Atomic Force Microscopy and Kelvin Probe Force Microscopy — ●JULIAN CREMER¹, SINAN KIREMIT², BERNHARD KALTSCHMIDT³, THOMAS KORDISCH², ANDREAS HÜTTEN³, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience (BINAS), Bielefeld University — ²Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences — ³Thin Films & Physics of Nanostructures, Bielefeld University

The pitting surface corrosion of three different stainless steels (1.4016, 1.4510 and 1.4301) used for industrial applications was investigated by exposition to oxidative liquids. Here, we focus on the investigation of the origin of the pitting using Kelvin probe force microscopy (KPFM) and on the prevention of corrosion by surfactants using high-resolution atomic force microscopy (AFM). KPFM allows to determine the work function of a sample with high spatial resolution. We found that the initiation of a pit can be caused by an abnormal anodic site (low work function) surrounded by a normal surface which acts as a cathode, or by the presence of an abnormal cathodic site (high work function) surrounded by a normal surface. In order to test whether KPFM can predict where and why pitting corrosion occurs, we use a micro corrosion liquid cell that allows live observation of the previously scanned area during corrosion. Additionally, we study the surface activity of surfactants acting as corrosion inhibitors on stainless steels regarding adsorption dynamics and layer thickness in different temperature-controlled solutions.

MM 18.17 Tue 17:30 P2

Reactive Surface Corrosion of Polypropylene studied with Atomic Force Microscopy — ●JULIAN CREMER¹, BERNHARD KALTSCHMIDT², ANDREAS HÜTTEN², and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience (BINAS), Bielefeld University — ²Thin Films & Physics of Nanostructures, Bielefeld University

The surface corrosion of various polypropylene samples used for industrial applications was investigated by exposition to oxidative liquids. The samples are formulated by different additive packages and include fillers such as talc or glass fibers for reinforcement. In particular, we study the aging and corrosion of these polypropylene samples in oxidative liquid media, analyzing the influence of temperature and oxidants. Contrary to aging induced by UV radiation, aging in oxidative liquids is rarely studied. Shedding some light on this research area, we placed the polypropylene samples in an oxidative test solution at 95°C, which was constantly renewed. In total, the samples were examined after ten different time steps up to 4000h. Mainly, we used atomic force microscopy (AFM) to image the samples and to determine the Young's modulus, which is a decisive parameter for the age of plastic materials. In some cases, we observe a growth of a fibrous structure on the surface covering nearly the whole sample. To determine the chemical composition of the bloomed structure and follow the aging on a chemical level, attenuated total reflection infrared spectroscopy was performed (ATR-FTIR). We present structural and chemical changes of aged industrial polypropylene as well as the consequence of additive blooming.

MM 18.18 Tue 17:30 P2

High-Pressure Torsion Deformed Magnesium: Microstructure Evolution and Hydrogen Diffusion — ●SABINE SCHLABACH^{1,2,3}, BINGYU WU¹, GIORGIA GUARDI¹, STEFAN WAGNER¹, JULIA IVANISENKO^{2,3}, and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology, Institute for Applied Materials, Karlsruhe, Germany — ²Karlsruhe Institute of Technology, Institute of Nanotechnology, Karlsruhe, Germany — ³Karlsruhe Institute of Technology, Karlsruhe Nano Micro Facility, Karlsruhe, Germany

Magnesium (Mg) is one of the materials considered as a solid state storage material for Hydrogen (H) as it is capable of storing up to 7.6 wt.% of H while forming magnesium hydride (MgH₂). However, the volume diffusion rate of H in MgH₂ is low, and thus the sorption rate of H is rather slow. As grain boundaries are suggested as fast diffusion paths, an increasing volume fraction of grain boundaries by reducing the grain size is aimed. Starting from polycrystalline bulk Mg, this can be done, e.g., by high-pressure torsion, one method of severe plastic deformation. The deformation induced microstructure evolution is investigated by using electron backscatter diffraction depending on different process parameters like imposed pressure and number of revolutions. Special attention is taken on local misorientations as a measure

of dislocation density and their possible influence on H-diffusion. The related H loading capability of the deformed Mg samples is tested at room temperature utilizing gas volumetry. In a first step, H-diffusion in the α -Mg phase is assessed as model system. Thus, the maximum H concentration is kept below the solid solution limit.

MM 18.19 Tue 17:30 P2

Co(OH)₂@FeCo₂O₄ as high-performance electrode material for supercapacitors — ●ZIDONG WANG^{1,2}, YUDE WANG², HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²School of Materials and Energy, Yunnan University, 6500504 Kunming, Peoples Republic of China

Spinel-type MCo₂O₄ (M = Zn, Ni, Fe, *) are regarded as a partial replacement of Co₃O₄ without crystal structure changes, and they provide advantages of lower cost and improved performance compared with Co₃O₄. Particularly, the variable valence of Fe in FeCo₂O₄ benefits the energy storage capability. However, previous works indicate that the attainable performance of FeCo₂O₄ is still limited. Herein, a 2D planar morphology design is proposed to optimize the performance of FeCo₂O₄ as active materials of supercapacitors. In this work, nano-sized Co(OH)₂ were composited on FeCo₂O₄ nanosheets skeleton by a simple one-step hydrothermal process. Due to the synergistic effect, the sample achieves outstanding performances with the specific capacitance of 1173.43 F g⁻¹ at a current density of 1 A g⁻¹ and 95.4% capacitance retention after 5000 cycles. It indicates that nanostructured Co(OH)₂@FeCo₂O₄ would have hopeful prospects in energy storage applications.

MM 18.20 Tue 17:30 P2

Quantitative investigation of reversible Li₂O formation on Germanium battery anodes — ●KE WANG and GUIDO SCHMITZ — Chair of Materials Physics, Institute for Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany

Lithium-ion batteries (LIB) serves as efficient energy storage devices in many aspects of our life. Anodes belonging to the Group IV (Si, Ge and Sn) are promising candidates to replace commercially applied graphite (372 mAh g⁻¹) owing to their high theoretical capacity (3850 mAh g⁻¹ for Si, 1570 mAh g⁻¹ for Ge, and 990 mAh g⁻¹ for Sn). But, the respective mechanisms of Li storage and the formation of solid electrolyte interface (SEI) are still not clearly. In this work, cyclic voltammetry has been conducted in combination with a quartz crystal microbalance to measure the SEI mass, and the amount of eventually reversibly processed species. Similar to Si and Sn, also with Ge anodes, the QCM mass spectroscopy identifies Li₂O as a reversibly processed species that contributes a significant part to the electrochemical capacity. The amount of reversibly stored Li₂O decreases weakly with increasing cycling rate, but increases significantly with the thickness of the Ge anodes. Interestingly, the amount of Li₂O decreases if pronounced anode cracking appears, which is probably attributed to the fact that the fracture introduces short circuit transport paths deep into the volume of the Ge which accelerates lithiation. Thermodynamically, Li₂O should form before Li is inserted. But in the experiment simultaneously formation of Li₂O and Li_xSn_y is observed on Sn, probably attributed to lateral heterogeneity introduced by surface roughness.

MM 18.21 Tue 17:30 P2

Recycling of anode graphite from spent lithium-ion batteries and reused in heat transfer medium — ●YU QIAO^{1,2}, ZHONGHAO RAO^{3,4}, HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²School of Electrical and Power Engineering, China University of Mining and Technology, 221116, Xuzhou, China — ³School of Energy and Environmental Engineering, Hebei University of Technology, 300401, Tianjin, China — ⁴Hebei Key Laboratory of Thermal Science and Energy Clean Utilization, Hebei University of Technology, 300401, Tianjin, China

Lithium-ion batteries (LIBs) have been widely employed in fast-growing mobile devices, stationary storage devices and electric vehicles. However, LIBs face a large wave of retirement because of a certain life. Graphite is the most common anode material in LIBs, amount of waste graphite will also be produced with the retirement of spent LIBs. Anode graphite (AG) from spent LIBs has the characteristics of large layer spacing and ease of being intercalated due to reducing the interlamination force after repeated charge and discharge cycles. In this study, two-dimensional graphite flakes (GFs) were prepared from spent AG through a freeze-thaw ultrasonic-assisted circulation method. The

heat transfer ability of as-obtained GFs dispersed in ethylene glycol was investigated experimentally. The results indicated that GFs could enhance the heat transfer coefficient and the maximum enhancement is about 30%.

MM 18.22 Tue 17:30 P2

Mild-temperature solution-assisted encapsulation of phosphorus into ZIF-8 derived porous carbon as lithium-ion battery anode — •CHENGZHAN YAN¹, SHUN WANG², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany. — ²Key Laboratory of Carbon Materials of Zhejiang Province, Institute of Materials and Industrial Technologies, Wenzhou University, Wenzhou, Zhejiang, 325027, China.

Phosphorus in the form of polyphosphides anions (PP) is encapsulated into ZIF-8 derived porous carbon through a solution-assisted etching diffusion process under a mild temperature, and the composites with a high phosphorous content of 30 wt% exhibit a high capacity, improved cycling stability as well as a good rate performance as a lithium-ion battery anode. Herein, a series of morphological and structural characterizations are applied to analyze the differences between individual MOF-derived carbon hosts with the whole body that has PP inside the pore. Subsequently, their electrochemical performance is also compared. The results of the above-mentioned material analysis and application practices jointly confirmed the superiority of this mild temperature solution-assisted encapsulation of phosphorus method. In summary, this work provides a new strategy to design and fabricate phosphorus-based electrodes for batteries beyond lithium-ion batteries.

MM 18.23 Tue 17:30 P2

Optimization of flash sintering input parameters for obtaining 8YSZ dense samples — •FÁBULO R. MONTEIRO¹, GUSTAVO C. DACANAL¹, JOÃO V. CAMPOS², LILIAN M. JESUS², ADILSON L. CHINELATTO³, and ELIRIA M. J. A. PALLONE¹ — ¹University of São Paulo, Pirassununga, Brazil — ²Federal University of São Carlos, São Carlos, Brazil — ³University of Ponta Grossa, Ponta Grossa, Brazil

Flash sintering has been widely investigated due to its technological potential, since it allows very rapid densification of different ceramic materials. The literature still lacks studies assessing how the electrical parameters of the technique (electric field and current density) involved in the process affect material densification since these parameters may vary depending on furnace type and, especially, sample geometry. Thus, this study used the response surface technique to analyze and relate, in a multivariate way, a few flash sintering variables. A mathematical model was proposed to optimize the densification of 8YSZ cylindrical and dog-bone samples. For this, a complete second order factorial planning with three central points was used in combination with the response surface methodology. The results obtained allowed us to predict electric field and electric current density values to optimize the densification of 8YSZ samples in the two geometries used and to understand how electric field and electrical current density values affected onset and sample temperatures (estimated by the black body radiation model).

MM 18.24 Tue 17:30 P2

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 — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 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 18.25 Tue 17:30 P2

Magnetic Hardening of Nd-Fe-B Permanent Magnets — •LUKAS SCHÄFER¹, KONSTANTIN SKOKOV¹, FERNANDO MACCARI¹, ILIYA RADULOV¹, DAVID KOCH², and OLIVER GUTFLEISCH¹ — ¹Functional Materials, Institute of Material Science, Technical University of Darmstadt, 64287, Darmstadt, Germany — ²Strukturforschung, Institute of Material Science, Technical University of Darmstadt, 64287, Darmstadt, Germany

Nd-Fe-B alloys used for permanent magnets provide highest performance and energy density and are therefore used in numerous energy and high-tech applications. The superior intrinsic properties of the hard magnetic Nd₂Fe₁₄B phase are translated by a controlled production processes leading to a specific micro- and grain boundary structure and high coercivity. In this work, we take a different approach and show a novel magnetic hardening mechanism in such materials. This mechanism has the potential to be incorporated into existing manufacturing processes and to be adapted to novel production routes for Nd-Fe-B permanent magnets such as Additive Manufacturing. As an example, we demonstrate how the microstructural transformation from metastable Nd₂Fe₁₇B_x phase to the hard magnetic Nd₂Fe₁₄B phase by controlled annealing leads to a significant increase in coercivity from 250 kAm⁻¹ to 700 kAm⁻¹ in Nd₁₆Fe_{bal-x-y-z}Co_xMo_yCu_zB₇ alloys. This approach offers also a promising opportunity for the fabrication of nano composite magnets.

MM 18.26 Tue 17:30 P2

Spin fluctuations and Wigner thermal transport in thermoelectric skutterudites — •ENRICO DI LUCENTE¹, MICHELE SIMONCELLI², and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne 1015, Switzerland — ²TCM Group, Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge, CB3 0HE UK

Skutterudites are highly promising functional materials due to their peculiar thermoelectric and magnetic properties. We elucidate the complex phenomenology that takes place in these materials both in terms of spin fluctuations and in the crossover from a Peierls-Boltzmann to a Wigner thermal transport regime, where tunneling of phonon wavepackets emerges. We first study the electronic structure using the state-of-the-art DFT+Hubbard theory to uncover multiple self-consistent magnetic and charge disproportionated configurations. While the lowest energy state is antiferromagnetic but metallic, paramagnetic fluctuations captured through a special quasi random structure open a small gap of 61 meV, in good agreement with experiments. Moreover, in going from the parent compound to the related filled skutterudite, a transition from a Peierls-Boltzmann to a Wigner thermal transport regime arises, where, at working temperature of the devices, the tunneling of phonon wavepackets becomes as relevant as the drifting diffusion.

MM 18.27 Tue 17:30 P2

Freezing and melting of water in nanopores: A temperature-dependent X-ray scattering study — •LARS DAMMANN^{1,2}, STELLA GRIES^{1,2}, MILENA LIPPMANN¹, and PATRICK HUBER^{1,2} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany — ²Hamburg University of Technology, Institute for Materials and X-Ray Physics, Eißendorfer Straße 42, Hamburg 21073, Germany

The crystallization of water in extreme spatial confinement of nanoporous media plays a pivotal role in many natural and technological processes, ranging from frost heave to modern materials processing. However, the induced interfacial stresses in the porous medium during melting and crystallization and the crystalline structures of nanoconfined water are still subject of scientific discussions. Here we present simultaneous temperature dependent small and wide angle X-ray scattering (SAXS/WAXS) measurements of water in ordered silica nanopores of diameters around 3 nm and 7-8 nm in a temperature range from 300 K to 150 K. With SAXS we investigate the crystallization induced strain on the pore network and with WAXS the structure of water ice in nanoconfinement. A complete analysis of the measurements is yet to be conducted, however, promising first results of the SAXS measurements show a strong dependence of pore strain on freezing in the pores especially for the smaller pores. As a next step we aim to compare the SAXS data to the measured WAXS signal to investigate the structure of the crystallized confined water.

MM 18.28 Tue 17:30 P2

Liquids in Atom Probe Tomography — ●TIM MAXIMILIAN SCHWARZ, HELENA SOLODENKO, JONAS OTT, GUIDO SCHMITZ, and PATRICK STENDER — University of Stuttgart, Institute for Materials Science, Chair of Materials Physics, Heisenbergstr. 3, 70569 Stuttgart, Germany

Frozen liquids are challenging and rather new in the investigation by atom probe tomography. However, recent progress in instrumentation, especially the introduction of cryo transfer shuttles, and the development of the required preparation routes to shape nanometric needles of frozen liquids enable measurements of sufficient quality and size of data sets to discover the typical features of this material class. The field evaporation of liquids resembles more the behaviour of weakly cross-linked polymers than that of metals. So frozen liquids, stabilized by weak hydrogen or van der Waals bonds, typically evaporate in large molecular fragments which raises general questions about spatial resolving power and chemical sensitivity of the atom probe tomography. At the example of saturated glucose solutions, we investigate the accuracy of the chemical analysis and the spatial resolution in localizing dissolved molecules. The direct comparison to the field evaporation of solid bulk glucose demonstrates in water a matrix-assisted field desorption that enables the detection of the chemical structure of larger organic molecules. One step further natural honey, which is a super-saturated solution consisting of a mixture of different monosaccharides and higher sugars in water, can be investigated on the nanoscale.

MM 18.29 Tue 17:30 P2

Fractal abnormal grain growth in nanocrystalline Pd-Au at the atomistic level — ●JOHANNES WILD¹, TORBEN BOLL¹, JULES DAKE², DOROTHÉE VINGA SZABÓ¹, STEFAN WAGNER¹, CARL E. KRILL², and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — ²University of Ulm, Institute of Functional Nanosystems, Ulm, Germany

Nanocrystalline (NC) Pd-10 at.% Au (PdAu) prepared by inert gas condensation (IGC) shows an unconventional manifestation of abnormal grain growth upon heat treatment. This unusual growth mode leads to complex and highly convoluted boundaries resembling those of fractal shapes. Furthermore, the microstructure shows a bimodal grain size distribution with regions of NC grains bordering grains in the micron range. This phenomenon is unique to this NC PdAu as conventionally prepared samples showed normal grain growth for the same heat treatment. In this study, we investigate the abnormal grain boundaries of heat-treated IGC PdAu using atom probe tomography (APT) and field ion microscopy (FIM). The position-specific APT samples are produced by targeted sample preparation with focused ion beam lift-out methods at chosen regions of interest that are identified beforehand by high-resolution electron backscatter diffraction imaging. We also use FIM, which has a higher lateral resolution than APT. This research is financially supported by the Deutsche Forschungsgemeinschaft (DFG) via project number 461632490, DFG PU131/18-1, DFG KR1658/10-1 and Karlsruhe Nano Micro Facility (KNMF).

MM 18.30 Tue 17:30 P2

Formation porous metal nanosystems under near-equilibrium condensation conditions in plasma-condensate system — ●ANNA KORNUSHCHENKO^{1,2}, VYACHESLAV PEREKRESTOV¹, and GERHARD WILDE² — ¹Sumy State University, Laboratory of Vacuum Nanotechnologies, Sumy, Ukraine — ²Westfälische Wilhelms-Universität, Institute of Materials Physics, Münster, Germany

It is known, that porous structures depending on morphology can possess unique physical properties which can determine areas of their application. In the proposed work a new technique for synthesizing metal porous micro- and nanostructures has been developed. This approach is based on the phase transition of sputtered substances into the condensed state under conditions close to thermodynamic equilibrium. The low dimensional metal systems (Cr, Zn, Cu, Ti, Ni, Al) have been obtained in the different morphological forms, such as network structures, nanowires, agglomerations of weakly-bound crystals, columnar structures consisting of prolonged crystals with approximately identical habitus, etc. The results confirm the important new opportunities for size, shape and physical property tuning of nanostructured materials that are given by deposition near thermodynamic equilibrium conditions. It has been established that the growth mechanism under conditions close to thermodynamic equilibrium possesses principally new peculiarities and possibilities in comparison with traditional meth-

ods of condensation from vapor state and consequently can contribute to a new zone in the structure zone model.

MM 18.31 Tue 17:30 P2

Self-detachment and sub-surface densification of dealloyed nanoporous thin films — ●GIDEON HENKELMANN¹, DIANA WALDOW¹, MAOWEN LIU¹, LUKAS LÜHRS¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — ²Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

This work highlights experimental observations showing microstructural gradients at interfaces in nanoporous gold, and it explains those observations as a consequence of gradients in a laterally averaged mean curvature of the pore surfaces. Nanoporous gold can be covered by a densified layer at its external surfaces. Furthermore, as we report, thin films of the material often spontaneously detach from massive gold base layers that are intended to enhance adhesion to the substrate. Those phenomena appear intrinsic to the material, as they are naturally reproduced by our kinetic Monte Carlo (KMC) simulation of dealloying and of the subsequent microstructure evolution. Our results suggest that spontaneous densification or decohesion at interfaces may be generic features of nanoscale porous network materials that evolve by curvature-driven surface diffusion.

MM 18.32 Tue 17:30 P2

Structural-mechanical property correlation in hierarchical nanoporous gold — ●LUKAS RIEDEL¹, SHAN SHI^{1,2}, JÜRGEN MARKMANN¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany — ²Institute of Material Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Implementing a structural hierarchy in nanoporous metals has been demonstrated as an efficient way to achieve lightweight and enhanced mechanical performance. So far, several aspects of the correlation between structure and mechanical behavior are not clearly proven. Here, hierarchical nanoporous gold (HNPG) with tunable ligament size at each hierarchy level is synthesized out of Ag90Au10 via a dealloying-coarsening-dealloying strategy. The structural analysis is conducted with scanning electron microscopy, small-angle X-ray scattering (SAXS) and ultra small-angle X-ray scattering (USAXS). We demonstrate that SAXS and USAXS are valued as advantageous methods for the determination of the structural size of HNPG. In particular, USAXS is very useful for the description of nanoporous structures with a ligament size of several hundred nanometers. It is observed that the mechanical behavior of HNPG is highly dependent on the ligament size at both the upper and the lower hierarchy level. Moreover, HNPG made out of Ag90Au10 shows improved stiffness in comparison to HNPG made out of Ag93Au7 even though they have similar feature sizes. The results represent an evidence for the development of the connectivity during coarsening in relation to the solid fraction.

MM 18.33 Tue 17:30 P2

Hierarchical-structural effect on creep of nanoporous gold — ●HANSOL JEON¹, SHAN SHI^{1,2}, JÜRGEN MARKMANN^{1,2}, and ERICA LILLEODDEN³ — Helmholtz-Zentrum Hereon, Institute of Materials Mechanics, 21502 Geesthacht — ²Hamburg University of Technology, Institute of Materials Physics and Technology, 21073 Hamburg — ³Fraunhofer Institute for Microstructure of Materials and Systems, 06120 Halle (Saale)

Nanoporous gold (NPG), a bi-continuous structure composed of ligaments and pores, is highly attracting attention in application fields due to its high surface area and chemical inertness. In addition, hierarchical nested-network nanoporous gold (N3PG) has been developed as an even lighter and faster functional material. With respect to mechanical properties, the research on the time-dependent deformation as called creep for NPG and N3PG is scarce while there have many studies of tension, compression, and nanoindentation. In this study, we performed compressive creep tests for NPG and N3PG pillars in order to investigate the creep behavior under control of the electrochemical potential. We prepared N3PG samples with the same higher-level ligament size and with different lower-level ligament-sizes and a non-hierarchical NPG sample according to the higher-level ligament size so that we analyzed the effect of lower-level ligament-size on N3PG as well as the effect of the hierarchical structure itself on creep. In addition, by controlling the electrochemical potential, we controlled the surface status in order to check on the size effect of the relationship

between creep behavior and surface state.

MM 18.34 Tue 17:30 P2

Fabrication of hierarchical porous silicon and amorphous silica by means of silver nanoparticle catalyzed chemical etching — ●STELLA GRIES^{1,2,3}, MANUEL BRINKER^{1,2,3}, and PATRICK HUBER^{1,2,3} — ¹Institute for Materials and X-Ray Physics, Hamburg University of Technology, 21073 Hamburg, Germany — ²Center for X-Ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — ³Center for Hybrid Nanostructures CHyN, University of Hamburg, 22607 Hamburg, Germany

Many biological tissues and materials exhibit a multiscale porosity with small, often nanoscale pores as well as large, macroscopic pores or capillaries in order to achieve simultaneously large inner surfaces in combination with an optimized mass transport capability. Achieving such a hierarchical porosity in artificial porous media is a very active research field. Here we present a novel approach based on silver nanoparticle-assisted chemical etching (MACE) of electrochemically fabricated macroporous silicon for the synthesis of wafer-scale, single-crystalline silicon with a bimodal pore size distribution. With MACE macroporous silicon membranes can be porosified into hierarchical porous silicon (hp-Si). The resulting semiconducting material offers good hydraulic permeabilities and simultaneously a large inner surface for potential applications in energy harvesting or conversion or for on-chip sensorics and actuorics. Finally, the hp-Si membranes can be transformed by thermal oxidation at temperatures above 800°C to hierarchical porous amorphous silica a material that could be of particular interest for opto-fluidic and photonic applications in the visible.

MM 18.35 Tue 17:30 P2

In situ X-ray spectroscopic and scattering studies on the emergence of CoO nano-assemblies in solution — ●CECILIA ZITO¹, LUKAS GROTE^{1,2}, KILIAN FRANK³, ANN-CHRISTIN DIPPPEL², PATRICK REISBECK³, KRZYSZTOF PITALA⁴, KRISTINA KVASHNINA⁵, STEPHEN BAUTERS⁵, BLANKA DETLEFS⁵, OLEH IVASHKO², PALLAVI PANDIT², MATTHIAS REBBER¹, SANI HAROUNA-MAYER¹, BERT NICKEL³, and DOROTA KOZIEJ¹ — ¹University of Hamburg, Germany — ²Deutsches Elektronen-Synchrotron, Hamburg, Germany — ³Ludwig-Maximilians-Universität München, Germany — ⁴AGH, University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland — ⁵European Synchrotron Radiation Facility ESRF, Grenoble, France

The key to fabricating complex, hierarchical materials is the control of chemical reactions at various length scales. The classical crystallization theory is insufficient to properly describe the chemical reaction leading to monomer formation, the evolution of small primary particles, and how they assemble into superstructures. Here, we illustrate how the combination of advanced X-ray spectroscopic and scattering in situ studies probe length scales all the way from atomic to macroscopic, and shed light on the formation mechanism of CoO nanocrystal assemblies in solution. Utilizing HERFD-XANES, we directly access the molecular level of the nanomaterial synthesis. We reveal that initially Co(acac)₃ rapidly reduces to square-planar Co(acac)₂ and coordinates to two solvent molecules. Furthermore, we track subsequent structural changes with in situ total X-ray scattering and atomic pair distribution function analysis, pinning down the transition from the dissolved Co complex to crystalline CoO. Ultimately, SAXS uncovers the assembly process of the crystallites into distinct spherical superstructures. The concomitant growth and assembly of crystallites into a superstructure differentiates the investigated pathway from a classical mechanism. The combination of X-ray spectroscopy and scattering can elucidate the emergence of assemblies in solution with a broad perspective.

MM 18.36 Tue 17:30 P2

Hierarchical materials mimicking mechanical behaviour of human bone synthesized by additive manufacturing and dealloying. — ●ALEKSANDR FILIMONOV¹, LUTZ MÄDLER^{1,2}, and ILYA OKULOV^{1,2} — ¹Faculty of Production Engineering, University of Bremen, Badgasteiner Str. 1, 28359 Bremen, Germany — ²Leibniz Institute for Materials Engineering-IWT, Badgasteiner Str. 3, 28359 Bremen, Germany

The close match between the elastic properties of an implant material and bone is crucial to avoid the stress-shielding effect. Therefore, low modulus biomaterials are desirable for biomedical implants that ensure rapid healing of hard tissue. Due to its complex hierarchical structure, bone features moderate strength similar to some metals and low elastic modulus like polymers. Implant materials for bone fixation should be

several times stronger compared with that of bone. However, the general relation between strength and elastic modulus of man-made materials suggest that stronger materials typically possess higher elastic modulus including metals - usual candidates for bone fixation. In this work, novel hierarchical metal-polymer composite materials "breaking" the general trend between strength and elastic modulus were synthesized by additive manufacturing and liquid metal dealloying. The large digital porosity of metallic scaffold was synthesized by additive manufacturing and its fine porosity is a result of materials self-organization upon dealloying. The results suggest that these novel composite materials mimicking the structure and mechanical behaviour of bone are potential candidates for biomedical applications.

MM 18.37 Tue 17:30 P2

Peculiarities of electron transport and resistive switching in point contacts on TiSe₂ and TiSeS. — DMYTRO BASHLAKOV¹, ●OKSANA KIVITNITSKAYA¹, YULIYA SHERMERLIUK², SAICHARAN ASWARTHAM², DMITRI EFREMOV², BERND BÜCHNER^{2,3}, and YURI NAIDYUK¹ — ¹B. Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine, Kharkiv, Ukraine — ²Institute for Solid State Research, IFW Dresden, Dresden, Germany — ³Institut für Festkörper- und Materialphysik und Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Dresden, Germany

We report resistive switching in voltage biased point contacts (PCs) based on the transition metals chalcogenides TiSe₂ and TiSeS. The switching is taking place between a low resistive *metallic-type* state and a high resistive *semiconducting-type* state by applying bias voltage (<0.4V), while reverse switching takes place by applying voltage of opposite polarity. The difference in resistance between these two states can reach of about two orders of magnitude at helium temperature. The origin of the effect can be attributed to the electric field induced change of stoichiometry in PC core due to drift of Se vacancies. Additionally, we demonstrated, that heating takes place in PC core, which can facilitate the electric field induced effect. At the same time we did not find any evidence for CDW spectral features in our PC spectra for TiSe₂. The observed resistive switching allows to propose TiSe₂ and TiSeS as the promising materials, e.g., for non-volatile resistive random access memory (ReRAM) engineering.

MM 18.38 Tue 17:30 P2

Electron-phonon interaction and point contact enhanced superconductivity in trigonal PtBi₂ — DMYTRO BASHLAKOV¹, ●OKSANA KIVITNITSKAYA¹, GRIGORY SHIPUNOV², SAICHARAN ASWARTHAM², OLEG FEYA^{2,3}, DMITRI EFREMOV², and BERND BÜCHNER^{2,4} — ¹B. Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine, Kharkiv, Ukraine — ²Institute for Solid State Research, IFW Dresden, Dresden, Germany — ³Kyiv Academic University, Kyiv, Ukraine — ⁴Institut für Festkörper- und Materialphysik und Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Dresden, Germany

PtBi₂ is a Weyl semimetal, which demonstrates superconductivity with low critical temperature T_c ~ 0.6 K in the bulk. Here, we report our study of electron-phonon interaction (EPI) in trigonal PtBi₂ by the Yanson point contact (PC) spectroscopy and presenting the observation of PC enhanced superconductivity. We show, that the Yansons PC spectra display a broad maximum around 15 meV, indicating, apparently, EPI mechanism of Cooper pairing in PtBi₂. Moreover, we discovered a substantial increase of T_c up to ~ 3.5 K in PCs. The observed T_c is sufficiently higher than the bulk value, as well as detected at hydrostatic pressure. We calculated the phonon density of states and Eliashberg EPI function in PtBi₂ within the framework of the density functional theory. A comparison of experimental data with theoretical calculations showed acceptable agreement. The theoretical T_c is 3.5 K, which corresponds to the experimental value.

MM 18.39 Tue 17:30 P2

Quantification of intrinsic surface charges on MgO nanocubes using off-axis electron holography — ●YAN LU^{1,2}, FENGSHAN ZHENG¹, QIANQIAN LAN¹, MICHAEL SCHNEEDLER¹, PHILIPP EBERT¹, and RAFAL E. DUNIN-BORKOWSKI¹ — ¹Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C 1) and Peter Grünberg Institute (PGI 5), Forschungszentrum Jülich, Jülich, Germany — ²Beijing Key Lab and Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing, China Metal oxide nanoparticles exhibit outstanding catalytic properties, believed to be related to the presence of oxygen vacancies at the particle

surface. However, little quantitative is known about concentrations of point defects inside and on surfaces of these nanoparticles due to the challenges in achieving an atomically resolved experimental access. By employing off-axis electron holography, we demonstrate exemplarily using MgO nanoparticles as a methodology, which allows us to discriminate between mobile charges induced by electron beam irradiation and immobile charges associated with deep traps induced by point defects as well as distinguish between bulk and surface point defects. Counting the immobile charges provides a quantification of the concentration of F^{2+} centers induced by oxygen vacancies at the MgO nanocube surfaces.

MM 18.40 Tue 17:30 P2

3D Printed One Piece Surface Alteration Sensor with Galvanic Isolation — ●MICHAEL FEIGE and SONJA SCHÖNING — Bielefeld Institute for Applied Materials Research (BifAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences and Mathematics

More recently it is possible to combine conductive and non-conductive materials in one 3D print process. This allows printing of complex structures like PCBs, 3D coils, transformers, capacitors or high frequency components like antennas or transmission lines. Furthermore it is possible to combine those components to build highly specialized sensors in one production step.

We developed a concept for a sensor which, in its specialized form, could be used for detection of mechanical, chemical or biological alteration of surfaces such as abrasion, material degradation or separation. The detection method is based on an electrical, inductive readout while maintaining a sufficient galvanic isolation between the sensing area and the readout circuit.

In this contribution an actual sensor device capable of detecting corrosion is presented, which was designed, printed and tested with successful results. The sophisticated design outweighs the lack of high electrical conductivity and high magnetic permeability within the range of printable materials by the ability of the printer to precisely integrate the conductive material into the insulating material.

MM 18.41 Tue 17:30 P2

A first study on the current-controlled flash sintering experiments on 3YSZ-Ni composites — ●PRANAV RAI and DEVINDER YADAV — Department of Metallurgical and Materials Engineering, Indian Institute of Technology Patna, Bihta, Patna 801106, India

Flash sintering involves densification of ceramic bodies in few seconds at relatively low furnace temperatures. The normal flash sintering experiments are characterized by a non-linear rise in the electrical conductivity of the sample. In the present work, flash sintering experiments were conducted in the current-controlled mode where the current is made to increase linearly through the sample at a constant rate. The sample sinters progressively as the current increases. Composites of 3YSZ and Ni, with different Ni contents (5wt.%, 10wt.%, and 20wt.%) were flash sintered at a constant current rate of 600 mA/min with a target current density of 100 mA/mm², at a furnace temperature of 900°C. The total span of the experiments was 50 s. The extent of densification decreased with increase in Ni content. In addition, the samples with higher Ni content started to densify at a higher current density. XRD revealed oxidation of Ni in all the samples, post flash sintering. However, complete oxidation of Ni to NiO in conventional

sintering of the same composites occurred at 1450°C after a hold time of 2 hours. The flash sintered microstructure of 3YSZ phase was characterized by relatively fine grains with narrow grain size distribution. The 3YSZ-20Ni samples exhibited a microstructure with percolating network of the NiO phase. The processed samples can have possible applications in designing the anode materials for solid oxide fuel cells.

MM 18.42 Tue 17:30 P2

Electrospun Electroluminescent CsPbBr₃ Fibers: Flexible Perovskite Networks for Light-Emitting Application — ●KHAN LÉ¹, FLORIAN VON TOPERCZER², FERAY ÜNLÜ¹, THOMAS FISCHER¹, KLAS LINDFORS², and SANJAY MATHUR¹ — ¹Institute of Inorganic Chemistry, University of Cologne, Greinstr. 6, 50939 Cologne, Germany — ²Institute of Physical Chemistry, University of Cologne, Greinstr. 4-6, 50939 Cologne, Germany

Organic-inorganic and all-inorganic lead halide perovskites (APbX₃) have continuously attracted research interest and went through significant improvements towards highly efficient photovoltaic technologies and LEDs. Most lead-halide perovskite devices are based on thin films or quantum dots while reports on alternative morphologies are scarce. We prepared CsPbBr₃@polymer composite nanofibers by one-step electrospinning and characterized them by scanning electron microscopy, transmission electron microscopy, X-ray diffractometry, UV/vis and photoluminescence spectroscopy. As a proof-of-concept, we subsequently integrated the fiber mats as active layers in electrically driven light emitting devices. While the synthesis of perovskite nanofibers is not new, to the best of our knowledge we would be the first to report on electroluminescence of such fibers. In addition, all preparations were conducted under ambient atmosphere and the perovskite precursor ink was prepared with low toxicity solvents (H₂O/EtOH/ionic liquid). This work could pave the way towards cost effective and flexible optoelectronic fiber- or yarn-based lead-halide perovskite devices by an up-scalable method.

MM 18.43 Tue 17:30 P2

Raman spectra of Arsenopyrite: Experiment and Theory — ●NEBAHAT BULUT¹, AYBERK ÖZDEN¹, CAMELIU HIMCINSCHI¹, ESTEBAN ZUNIGA PUELLES², ROMAN GUMENIUK², and JENS KORTUS¹ — ¹TU Bergakademie Freiberg, Institute of Theoretical Physics — ²TU Bergakademie Freiberg, Institute for Experimental Physics, Germany

Arsenopyrite (FeAsS) is a semiconductor with a small bandgap and a common source for arsenic (As) mineral. Chemical and structural information on this material is still of interest. The crystal structure is, monoclinic with space group P2₁/c, derived from orthorhombic marcasite (FeS₂) [1]. Here we present a combined experimental and theoretical study on the vibrational properties of arsenopyrite, which have to our knowledge not yet been reported. Raman spectra have been recorded experimentally by means of a LabRam HR800 spectrometer from HORIBA Jobin Yvon using 633 nm laser as the excitation source. Additionally, Raman spectra were calculated using Quantum Espresso [2] with norm-conserving pseudopotential and PZ exchange-correlation functional. The comparison of experimental and theoretical data shows good agreement and allows for symmetry assignment of the Raman peaks.

[1] Bindi, L.; Moelo, Y.; Leone, P.; Suchaud, M. *Can. Mineral.* 50, 471*479 (2012).

[2] P. Giannozzi et al., *J.Phys. Condens. Matter* 21, 395502 (2009)

MM 19: Invited Talk Fritz Körmann

Time: Wednesday 9:30–10:00

Location: H44

Invited Talk MM 19.1 Wed 9:30 H44
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 20: Computational Materials Modelling: HEA, Alloys & Nanostructures

Time: Wednesday 10:15–13:00

Location: H44

MM 20.1 Wed 10:15 H44

Microstructural evolution of severely deformed nanocomposite high entropy alloys irradiated by swift heavy ions

— ●SHABNAM TAHERINIYA¹, CHRISTIAN GADELMEIER², HARALD RÖSNER¹, MARTIN PETERLECHNER¹, CHRISTOPH GAMMER³, MARILENA TOMUT^{1,4}, SERGIY V. DIVINSKI¹, UWE GLATZEL², and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Germany — ²Metals and Alloys, University of Bayreuth, Bayreuth, Germany — ³Erich Schmid Institute of materials Science, Austrian Academy of Science, Leoben, Austria — ⁴GSF Helmholtz Center for Heavy Ion Research, Darmstadt, Germany

Structural modifications induced by the processing of high entropy alloys (HEAs) under non-equilibrium conditions are investigated to shed light into the stability of such advanced materials. The nanocomposite HEAs are produced by the room-temperature high pressure torsion (HPT) of stacked single-phase equiatomic FCC CoCrFeMnNi (Cantor) and BCC HfNbTaTiZr (Senkov) alloys. Solely Cantor and Senkov alloys were HPT-processed under the similar conditions, too. Cross-sections of the HPT-processed disks were subjected to high fluences of Au swift-heavy-ion irradiation at ambient and cryogenic temperatures. Deformation and irradiation-induced microstructural changes were examined in detail applying scanning and transmission electron microscopies with respect to evolution of chemical composition and local microstructure. A combination of nano-beam diffraction with angular correlation was utilized to provide information about the resolved crystal structures and strain fields in the different HEA phases.

MM 20.2 Wed 10:30 H44

Impact of high-pressure torsion and post-deformation annealing on CoCrFeMnNi high-entropy alloy with carbon content

— ●SANDRA HECHT, SERGIY V. DIVINSKI, and GERHARD WILDE — Institute of Materials Physics, University of Münster, Münster, Germany

The well-known Cantor alloy CoCrFeMnNi provides attractive mechanical properties and strength-ductility combinations, which can be improved by further alloying of small amounts of carbon.

In the present work, the impact of high-pressure torsion (HPT) and post-deformation annealing on equiatomic Cantor alloy and nearly-equiatomic (C alloyed (4.4 at.%) Cantor alloy, produced via arc-melting and subsequent homogenization at 1373 K for 3 days under pure Ar, is examined. The thermal, mechanical and microstructural properties of the initially coarse-grained samples were investigated before and after deformation at room temperature (5 rotations at 8 GPa) and afterwards post-deformation annealing treatments using differential-scanning calorimetry (DSC), X-ray diffraction (XRD), scanning and transmission-electron microscopy (SEM & TEM) as well as micro-hardness measurements. Impact of the interstitial carbon and in particular the carbides Cr₂₃C₆ on the mechanical response and microstructure evolution is examined.

MM 20.3 Wed 10:45 H44

Phase Stability and Ordering in Ta-Mo-Cr-Ti-Al Refractory High Entropy Alloys — ●YILUN GONG¹, ALEXANDER SHAPEEV², FRITZ KOERMANN^{1,3}, and JOERG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Germany — ²Skolkovo — ³Delft University of Technology, The Netherlands

Predictive capabilities of phase stability and ordering in multi-component systems are critical to designing better alloys. This is particularly important for properties which are difficult to be quantified by traditional experimental techniques.

In the present work, a class of body-centered-cubic (bcc) refractory high entropy alloys was studied. In contrast to its superior high-temperature behaviour, it shows less-satisfying ductility below 600 °C. As origin of the poor mechanical performance long-range B2-ordering at low temperatures has been proposed but is still controversially discussed due to contradicting experimental findings. To predict and to quantify the temperature-dependent stable structure, we employed on-lattice machine-learning interatomic potentials (namely low-rank potentials). This type of potentials is capable of accurately describing chemical interactions in multi-component systems used in subsequent Monte Carlo simulations. Systematic studies of training qualities, statistical uncertainties and impact of local lattice distortions were con-

ducted. Computed ordering sequence, site occupancies, short-range order parameters and alloying with interstitial O will be discussed.

MM 20.4 Wed 11:00 H44

Stabilities and Mechanical Properties of Mg-based Light Metal Multi-Principal Alloys — ●WERNFRIED MAYR-SCHMÖLZER¹, JOHANNES KIRSCHNER², CLEMENS SIMSON⁴, CHRISTOPH EISENMENGER-SITTNER², JOHANNES BERNARDI³, and GREGOR VONBUN-FELDBAUER¹ — ¹Institute of Advanced Ceramics, TU Hamburg — ²Institute of Solid State Physics, TU Vienna — ³USTEM, TU Vienna — ⁴LKR, 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 mainly contain heavy d-Orbital metals, and investigations into low density light metal CCAs have been rare due to the complex binding modes of their constituents.

We use both a Cluster Expansion approach with stochastic pre-screening steps and neural network based pair potentials to scan the large configuration space of the Mg-Al-Cu-Zn system for stable phases. Training data was generated using DFT calculations implemented in the VASP code. In conjunction with experiments, we find that addition of Cu into the Al-Mg-Zn system inhibits phase separation by formation of a stable cubic phase, reflected in an increase of the calculated bulk modulus. Furthermore, we evaluate the predictive power of these screening methods and their ability to provide insights into simulation of physical properties of these complex multicomponent alloys.

MM 20.5 Wed 11:15 H44

In-situ Nanoalloying by Laser Powder Bed Fusion: Molecular Dynamics Simulations of Cantor-Alloy Formation in a Powder Blend — ●YULIA KLUNNIKOVA¹, ARNE J. KLOMP², and KARSTEN ALBE³ — ¹klunnikova@mm.tu-darmstadt.de — ²klomp@mm.tu-darmstadt.de — ³albe@mm.tu-darmstadt.de

Laser powder bed fusion (LPBF) is an additive manufacturing technology involving a gradual build-on of layers to form a complete component typically starting with prealloyed particles. Alternatively, one can also start with a powder blend and initiate in-situ alloying by the laser beam. In this context, multi-component systems, including high entropy alloys, are of particular interest. In this contribution we show results of molecular dynamics simulations of high-entropy nanoalloys formed by LPBF. We use the Cantor alloy as model system and explore the possibility to create the FeCrCoMnNi alloy from powder blends under far-from-equilibrium conditions and compare to the case of pre-alloyed nanopowders. By varying parameters (temperature field, melt pool, substrate type, etc.) we explore the correlation to microstructural features. In the case of the powder blend the elemental components mix in the liquid phase and solidify partially in crystalline and glassy states. Depending on the parameters of the laser (irradiation temperature, laser spot size) we see varying amounts of crystal defect, such as stacking faults, twinning, and vacancies. The results show that the resulting structures are delicately depending on the interplay of laser parameters, heat transport, interdiffusion and geometric factors. We acknowledge the NHR4CES for the computing time.

MM 20.6 Wed 11:45 H44

Phase stability and formation energies of stacking faults in intermetallic Mg_xAl_{2-x}Ca Laves phases — ●ALI TEHRANCHI, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max Planck institute for Iron research, Max Planck Straße 1, 40237 Düsseldorf

The intermetallic Laves phases that form in Mg-based alloys at higher alloying concentrations have a significant impact on their mechanical properties. For example, they can enhance the creep resistance of the alloys and extend their application to higher temperature domains. However, the mechanisms of deformation of these phases are not fully understood. In this work, at first the formation energies of the different realizations of C14, C15, and C36 Laves phases in the composition domain, Mg_xAl_{2-x} with 0 < x < 2, using the ab initio simulations is

15 min. break

15 min. break

MM 20.6 Wed 11:45 H44

Phase stability and formation energies of stacking faults in intermetallic Mg_xAl_{2-x}Ca Laves phases — ●ALI TEHRANCHI, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max Planck institute for Iron research, Max Planck Straße 1, 40237 Düsseldorf

The intermetallic Laves phases that form in Mg-based alloys at higher alloying concentrations have a significant impact on their mechanical properties. For example, they can enhance the creep resistance of the alloys and extend their application to higher temperature domains. However, the mechanisms of deformation of these phases are not fully understood. In this work, at first the formation energies of the different realizations of C14, C15, and C36 Laves phases in the composition domain, Mg_xAl_{2-x} with 0 < x < 2, using the ab initio simulations is

calculated. Using these formation energies, the phase diagram of the phases of interest is constructed. The effect of the strain fields on the relative stability of these phases is included. In addition, using the analytic Axial Next-Nearest Neighbor Ising (ANNNI) type model, the basal stacking faults in each phase and composition are calculated. The results of the analytic models are in good accordance with the results of the direct DFT simulations of the stoichiometric stacking faults. The gamma surface of certain realizations of the C36 phase is also investigated and explain the experimentally observed planar defects in the C36 phase.

MM 20.7 Wed 12:00 H44

Rational design of bimetallic nanoparticles — ●SAMUEL BALTAZAR^{1,2}, JAVIER ROJAS^{1,2}, PAMELA SEPULVEDA², and RAFAEL FREIRE² — ¹Physics Department, Universidad de Santiago de Chile, Chile — ²Center for the development of Nanoscience and Nanotechnology, Universidad de Santiago de Chile, Chile

The study of bimetallic nanoparticles (BNP) has recently attracted increasing attention from researchers worldwide due to their potential for technological applications in the electronic and environment fields. This study will be carried out through a theoretical framework to identify the fundamental atomic-scale mechanisms for BNP such as FeCu, AgCu, and FeNi. It is therefore necessary to determine the structural, electronic, and magnetic properties of the nanostructures with two or more elements, where the interplay between both metallic elements can be used to limit the oxidation of iron or the electron transfer between elements. This can be done based on some of the characteristics of these systems, such as (i) the surface-volume ratio, (ii) the shape of nanoparticles as an interesting aspect due to the physico-chemical properties at their surface, (iii) Concentration and (iv) distribution of elements. We performed molecular dynamics simulations under the NVT canonical ensemble to further deepen our study. The results pointed out that AgCu and FeNi BNP with a core shell and janus like morphologies are some of the most stable configurations, with a competition between them for FeCu as a function of the concentration and size of each element. These results were compared with experimental data for BNP, evidencing a good agreement among these approaches.

MM 20.8 Wed 12:15 H44

Atomic cluster expansion for the Ag-Pd system — ●YANYAN LIANG, MATOUS MROVEC, YURY LYSOGORSKIY, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Germany

Alloys of noble metals, such as silver and palladium, have been regaining attention in recent years due to their importance in nanotechnology and catalysis. However, for the binary Ag-Pd system reliable and efficient interatomic potentials that provide an accurate description of structural and thermodynamic properties are lacking. In this work, we developed a new atomic cluster expansion (ACE) parametrization for both elements Ag and Pd as well as their binary compounds by fitting to a large training set of ab initio data. The resulting ACE potential provides an accurate description for a wide range of fundamental properties, including the equations of states of various phases, elastic moduli, phonon frequencies, transformation paths, and defect energies. The excellent computer efficiency and linear scaling of ACE enable to

carry out large-scale molecular dynamics and Monte Carlo simulations to evaluate complex phenomena, such as thermal expansion, melting, diffusion and phase diagrams. Examples of these simulations will be provided to demonstrate the outstanding predictive power of ACE.

MM 20.9 Wed 12:30 H44

Atomistic modelling of hybrid organic-inorganic nanocomposites — KAI SELLSCHOPP¹, WERNFRIED MAYR-SCHMÖLZER¹, ROBERT MEISSNER², and ●GREGOR VONBUN-FELDBAUER¹ — ¹Institute of Advanced Ceramics, TU Hamburg, Germany — ²Institute of Polymers and Composites, TU Hamburg, Germany

Novel hybrid materials like supercrystalline nanocomposites from nano-building blocks promise excellent properties and functions for diverse applications. One realization are inorganic nanoparticles (NP) from transition-metal oxides which are functionalized with organic ligands and then assembled on different levels of hierarchy. In this contribution atomistic modelling based on density functional theory (DFT) calculations is used to shed light on the first level of hierarchy. Particularly, the interfacial properties of different ligands and effects in the interphase between the NP are addressed. For modelling interfaces, the configuration space is a challenge and here the program CodeRed (Configuration space determination and Reduction) is presented which allows to sample the adsorption configuration space and to select configurations as input for DFT calculations using unsupervised machine learning approaches. The results are further facilitated to obtain mechanical properties using DFT, and as input for molecular dynamics simulations as a first step towards multi-scale modelling to allow for an accurate description of larger and more complex systems.

MM 20.10 Wed 12:45 H44

Ab initio investigation of Mg alloy corrosion in water — ●JING YANG, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Magnesium alloys have great potential as structural materials for the automotive and aerospace industries, as well as bio-implants due to their low density and non-toxic nature. However, intrinsically poor ductility and poor corrosion resistance limit their practical application. In this work, we focus on the solid solution of Al and Ca in Mg, an alloying system which has shown improved ductility and corrosion resistance. In particular, we elucidate the effect of Al and Ca alloying on the aqueous corrosion process of Mg metal by ab initio molecular dynamics simulation of the metal/water system. We analyze the segregation behavior of the alloying elements, their impact on the interfacial water structure and dynamics, and the subsequent implication on corrosion kinetics. By combining our DFT calculations with thermodynamics, we construct interface phase diagrams for the Mg-Al-Ca system to elucidate the influence of the environment on surface structure and composition. We consider both implicit and explicit water calculations, which allows us to analyze the impact the water-modelling approach has on the constructed interface phase diagrams. We show that such ab initio molecular dynamics studies strongly improve our understanding on microscopic corrosion processes at realistic conditions.

MM 21: Transport in Materials: Thermal transport

Time: Wednesday 10:15–13:00

Location: H45

MM 21.1 Wed 10:15 H45

Computational modeling of extremely anisotropic van der Waals thermal conductors — SHI EN KIM¹, FAUZIA MUJID¹, AKASH RAI², ●FREDRIK ERIKSSON³, JOONKI SUH¹, PREETI PODDAR¹, ARIANA RAY⁴, CHIBEOM PARK¹, ERIK FRANSSON³, YU ZHONG¹, DAVID A. MULLER⁴, PAUL ERHART³, DAVID G. CAHILL², and JIWOONG PARK¹ — ¹Uni. of Chicago, USA. — ²Uni. of Illinois UC, USA. — ³Chalmers, Sweden. — ⁴Cornell Uni., USA.

Materials with thermal conduction anisotropy can provide innovative thermal management strategies in integrated circuits. However, artificially engineered material lacks the anisotropy ratios seen in nature. Here, we report extremely anisotropic thermal conductors based on large-area van der Waals thin films with random interlayer rotations, which produce a room-temperature thermal anisotropy ratio close to 900 in MoS₂, one of the highest ever reported. This is enabled by the

interlayer rotations that impede the through-plane conductivity, while the long-range intralayer crystallinity maintains high in-plane conductivity. In this contribution we will present the computational analysis of the measured ultralow thermal conductivities in the through-plane direction for MoS₂ (57 ± 3 mW m⁻¹ K⁻¹). Using molecular dynamics simulations we quantitatively explain these values and reveal a one-dimensional glass-like thermal transport. Conversely, the in-plane thermal conductivity in these MoS₂ films is close to the single-crystal value. Our work establishes interlayer rotation in crystalline layered materials as a new degree of freedom for engineering-directed heat transport in solid-state systems. Nature 597, 660-665 (2021)

MM 21.2 Wed 10:30 H45

Searching and Finding Thermal Insulators via ab initio Green-Kubo Simulations — ●FLORIAN KNOOP^{1,2}, THOMAS A.R. PURCELL¹, MATTHIAS SCHEFFLER¹, and CHRISTIAN CARBOGNO¹ —

¹The NOMAD Laboratory at the FHI-MPG and HU, Berlin, Germany — ²Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

We present a first-principles search for thermal insulators in material space, covering hundreds of compounds in seven space groups, including simple rocksalt and zinc blende structures up to complex perovskites. Using the high-throughput framework *FHI-vibes* [1] and a recently developed measure for the strength of anharmonicity, [2] we identify 120 experimentally known materials with potential for ultra-low thermal conductivity <2 W/mK at room temperature, i.e., comparable to those of thermoelectrics such as SnSe. For the 60 most promising candidates, we perform non-perturbative, fully anharmonic *ab initio* Green-Kubo simulations [3] to include all anharmonic effects. Besides revealing seven ultra-insulating compounds, these calculations shed light on the importance of strong anharmonic effects not accessible in perturbative phonon formalisms, e.g., short-lived metastable configurations and precursors of phase transitions.

[1] F. Knoop *et al.*, *J. Open Source Softw.* **5**, 2671 (2020).

[2] F. Knoop *et al.*, *Phys. Rev. Mater.* **4**, 083809 (2020).

[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

MM 21.3 Wed 10:45 H45

A spatially resolved optical method to measure thermal diffusivity — ●FEI SUN¹, SIMLI MISHRA¹, PHILIPPA H MCGUINNESS¹, ZUZANNA H FLIPIAK¹, IGOR MARKOVIC¹, DMITRY A SOKOLOV¹, NAOKI KIKUGAWA², JOSEPH W ORENSTEIN^{3,4}, SEAN A HARTNOLL⁵, ANDREW P MACKENZIE^{1,6}, and VERONIKA SUNKO^{1,3} — ¹Max Planck Institute, CPFS, Dresden, Germany — ²NIMS, Ibaraki, Japan — ³UC Berkeley, California, USA — ⁴LBNL, California, USA — ⁵Univ. of Cambridge, Cambridge, UK — ⁶Univ. of St Andrews, St Andrews, UK

We introduce an optical method to directly measure thermal diffusivity across a broad range of temperatures. Two laser beams are used, one as a source to locally modulate the temperature, and the other as a probe of the reflectivity. Thermal diffusivity is obtained from the phase delay between two beams. Combining the technique with a microscope setup allows for spatially resolved measurements. The in-plane diffusivity can be obtained when overlapping the two laser beams instead of separating them in the traditional way, which further enhances the spatial resolution. We demonstrate on two rutheranates: Sr₃Ru₂O₇ and Ca₃Ru₂O₇. The spatial resolution allowed us to study the diffusivity in single domains of the latter, and we uncovered a temperature-dependent in-plane diffusivity anisotropy. Finally, we used the enhanced spatial resolution to study the Ti-doped Ca₃Ru₂O₇. We observed large variations of transition temperature over the same sample, originating from doping inhomogeneity, and pointing to the power of spatially resolved techniques in accessing inherent properties.

MM 21.4 Wed 11:00 H45

Investigation of temperature dependent thermal transport in Sr₂RuO₄ and Sr₃Ru₂O₇ over a wide temperature range — FEI SUN¹, ●SIMLI MISHRA¹, ULRIKE STOCKERT¹, RAMZY DAOU², NAOKI KIKUGAWA³, ROBIN S PERRY⁴, SEAN A HARTNOLL⁵, ANDREW P MACKENZIE^{1,6}, and VERONIKA SUNKO^{1,7} — ¹Max Planck Institute - CPFS, Dresden, Germany — ²CRISMAT, ENSICAEN, UNICAEN, Normandie Université, Caen, France — ³NIMS, Ibaraki, Japan — ⁴LCN, University College London, London, UK — ⁵DAMTP, University of Cambridge, Cambridge, UK — ⁶School of Physics and Astronomy, University of St. Andrews, UK — ⁷Department of Physics, University of California, Berkeley, USA

We use optics to study thermal transport by modifying a typical laser pump-probe technique. A direct measurement of thermal conductivity is very challenging at high temperatures. In contrast, our method measures temperature dependent diffusivity over a wide range of temperature (10K up to 330K). As thermal diffusivity is the ratio of the thermal conductivity to the heat capacity, we can access the higher temperature thermal conductivity by an optical measurement of diffusivity and standard heat capacity measurement. We have used this technique to measure thermal diffusivity of two strongly correlated metals, Sr₂RuO₄ and Sr₃Ru₂O₇. This temperature dependent thermal transport combined with the resistivity measurements offers an insight into the electronic and phononic contributions to the quasiparticle scattering.

MM 21.5 Wed 11:15 H45

Simultaneous measurement for the complete characterization

of thermoelectric materials - real experiment and its digital twin — ●SEVERIN KOPATZ¹, ECKHARD MÜLLER^{1,2}, and PAWEŁ ZIOLKOWSKI¹ — ¹Institute of Materials Research, German Aerospace Center, Cologne, Germany — ²Institute of Inorganic and Analytical Chemistry, Justus Liebig University Gießen, Gießen, Germany

Thermoelectric (TE) materials directly convert thermal energy into electric energy. Their efficiency depends on the figure of merit zT ($zT = S^2\sigma/\kappa$). Commonly, the individual transport properties, mainly the electrical conductivity (σ), the Seebeck coefficient (S), and the thermal conductivity (κ) are measured in separate measurement set-ups. Here, we report on the 'Combined ThermoElectric Measurement' (CTEM) apparatus, which provides temperature-dependent measurements of the aforementioned transport properties on a single TE sample such as Co-doped FeSi₂ simultaneously. The measurements are carried out in a temperature range between room temperature and 600 °C. Since experimental CTEM results deviate from reference values, we introduce a digital twin of the CTEM. In combination with the real experiment, the numerical model allows to study possible error sources. One of the examples discussed in this talk concerns radiative effects which have to be considered especially at high temperatures above 300 °C and affect the measurement of the thermal conductivity in particular.

15 min. break

MM 21.6 Wed 11:45 H45

Appearance of non-equilibrium grain boundaries in additively manufactured high-entropy CoCrFeMnNi alloy — ●NURI CHOI^{1,2}, VLADISLAV KULITCKII¹, JOSUA KOTTKE¹, BENGÜ TAS¹, JUNGHOO CHOE³, JI HUN YU³, SANGSUN YANG³, JOO HYUN PARK², JAI SUNG LEE², GERHARD WILDE¹, and SERGIY DIVINSKI¹ — ¹Institute of Material Physics, University of Münster, Germany — ²Dep. of Mat. Sci. & Chem. Eng., Hanyang University, South Korea — ³Center for 3D Printing Materials Research, KIMS, South Korea

Additive manufacturing process with laser melting includes the repetitive melting/solidification, which generates residual thermal stresses in the bulk material, alongside with creation of various defects, including point defects, dislocations and numerous grain boundaries. How far the kinetic properties of these interfaces are modified by the processing remains an open issue, that is of fundamental importance for such phenomena as creep, phase transformation and precipitation. In the present study, grain boundary diffusion in additively manufactured CoCrFeMnNi high-entropy alloys is measured using the radiotracer technique. Since the additive manufacturing results in a hierarchical microstructure, grain boundary diffusion is examined in different samples prepared via different scan/build strategies. A non-equilibrium state of a fraction of high-angle grain boundaries is discovered. The non-equilibrium state is shown to relax after annealing at low temperatures without measurable microstructural changes. The grain boundary diffusivities of the 3D printed alloys are discussed with respect to those for fully homogenized cast or severe plastically deformed alloys.

MM 21.7 Wed 12:00 H45

Grain boundary diffusion and segregation of Cr in high-purity Ni bi-crystals with a $\Sigma 11$ grain-boundary — ●D. GAERTNER¹, S. V. SEVLIKAR¹, G. M. MURALIKRISHNA¹, D. COZLIN², D. IRMER², D. SCHREIBER³, B. TAS¹, M. VAIDYA¹, T. BRINK⁴, V. E. ESIN², C. DUHAMEL², G. DEHM⁴, V. RAZUMOSKII³, G. WILDE¹, and S. V. DIVINSKI¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²MINES ParisTech, PSL University, Centre des Matériaux, Évry, France — ³Materials Center Leoben Forschung GmbH (MCL), Austria — ⁴Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain-boundary diffusion of Cr in a Ni near $\Sigma 11(113)[110]$ bi-crystal is measured in an extended temperature interval between 503 K and 1303 K using the radiotracer technique. The grain boundary diffusion coefficients, D_{gb} , and the triple products, P are determined in the C- and B-type kinetic regimes, observing a strong deviation from the otherwise linear Arrhenius-type temperature dependence above 1000 K. The present results substantiate that the segregation factor of Cr in Ni is about unity, being in agreement with the preliminary findings in polycrystalline counterparts measured by SIMS and are fully supported by DFT-based calculations. Extensive MD simulations with empirical interatomic potentials substantiate an extreme stability of the $\Sigma 11$ grain-boundary structure in Ni from 0 K up to melting point. The non-linear Arrhenius temperature dependence is interpreted in terms of pronounced anharmonic contributions to defect formation at

elevated temperatures.

MM 21.8 Wed 12:15 H45

grain boundary melting phase transition in Ni-Bi system — ●BAIXUE BIAN¹, BORIS STRAUMAL², SERGIY DIVINSKI¹, and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Chernogolovka

Grain boundary segregation may drastically decrease the strength of structural materials. The intermediate temperature embrittlement of Ni-based alloys is a classical example of a catastrophic matrix degradation caused by solute segregation, in particular by Bi. In this work, the impact of grain boundary segregation of Bi in dilute polycrystalline Ni-Bi alloys on Ni grain boundary diffusion was systematically studied as function of temperature and composition. The radiotracer technique was used applying the ⁶³Ni radioisotope and measuring grain boundary diffusion in both B- and C-type kinetic regimes after Harrison's classification. An abrupt increase of the grain boundary diffusivities by about two orders of magnitude was observed at certain Bi contents which are unequivocally in the single-phase region of the corresponding bulk phase diagram. The present results unambiguously prove the occurrence of a pre-melting grain boundary phase transition in the Ni-Bi system.

MM 21.9 Wed 12:30 H45

Investigation of Phase Transitions in Polycrystalline Tungsten Trioxide Films during Ion Insertion and Extraction by in Situ Transmission and Raman Spectroscopy — ●MARKUS S. FRIEDRICH^{1,2}, ALEXANDER G. STRACK^{1,2}, PAUL K. TUCHECKER^{1,2}, JAN L. DORNSEIFER^{1,2}, and PETER J. KLAR^{1,2} — ¹Institute of Experimental Physics I, Giessen, Germany — ²Center for Materials Research, Giessen, Germany

The International Energy Agency stated in its "European Union 2020 Energy Policy Review" that in 2016 in the European Union alone 152 TWh were consumed for air conditioning (AC), despite only six per-

cent of the global stock of AC units is operated in the EU. So called "smart windows", e.g. windows based on electrochromic materials, such as tungsten trioxide, are promising candidates to reduce this kind of energy consumption. The coloration and bleaching of the EC material is based on the reversible insertion and extraction of small ions inside the material. Ion diffusion plays a key role in this process and therefore needs to be understood in depth in order to enable the optimization of future devices. Burkhardt et al. found, that the diffusion coefficient in this material is dependent on the concentration of already incorporated ions. We suggest, that this originates from changes in the crystal structure of the thin films. To substantiate this suggestion spatially and temporally resolved in situ transmission and Raman spectroscopic experiments were performed during potentiostatic ion insertion and extraction to correlate the diffusion of small ions inside the material with changes of its crystal structure.

MM 21.10 Wed 12:45 H45

Self-diffusion in ge2sb2te5 thin films — ●QINGMEI GONG, SERGIY DIVINSKI, and GERHARD WILDE — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-str. 10, 48149 Münster, Germany

Phase change memory devices (PCM) are considered as one of the most mature technologies among the emerging non-volatile memories and are based on the reversibility of the amorphous-to-crystalline transition within a nanosecond timescale. Ge₂Sb₂Te₅ is the most widely studied composition. In this work, the self-diffusion in Ge₂Sb₂Te₅ thin films is measured using secondary ion mass spectroscopy (SIMS) and applying the highly enriched natural ¹²²Te isotope. A 200 nm thick layer of Ge₂Sb₂Te₅ was deposited on a Si substrate by DC magnetron sputtering at room temperature. Subsequently, a thin layer of ¹²²Te was deposited on as-prepared Ge₂Sb₂Te₅/Si samples using physical vapor deposition. In the as-deposited state, Ge₂Sb₂Te₅ was amorphous as confirmed by XRD and transmission electron microscopy. The Te diffusion coefficients in Ge₂Sb₂Te₅ were estimated from SIMS measurements after annealing at different temperatures below crystallization onset.

MM 22: Data Driven Materials Science: Experimental Data Treatment and Machine Learning

Time: Wednesday 10:15–13:00

Location: H46

Topical Talk

MM 22.1 Wed 10:15 H46

Ingredients for effective computer-augmented experimental materials science — ●CHRISTOPH T. KOCH, MARKUS KÜHBACH, SHERJEEL SHABIH, BENEDIKT HAAS, and SANDOR BOCKHAUSER — Humboldt-Universität zu Berlin, Department of Physics & IRIS Adlershof, Berlin, Germany

Experimentally exploring the properties and uses of materials and improving them for particular purposes has been a major driving force for advancing the way people live over the last millennia. Experimental materials characterization techniques have now reached the level of detail that makes them converge with ab-initio computations based on fundamental building blocks: atoms and the electrons they share. During the last decades computers have surpassed the capacity of humans in the extraction of patterns in large amounts of data. It is thus a very natural consequence to involve their strengths also in further accelerating experimental materials science. In this talk we will use modern transmission electron microscopy as an example to illustrate current and future ways of how the process of linking the properties of materials to their fundamental structure can be supported computationally and by the availability of FAIR experimental and theoretical data sets. Along the way the contributions of the NFDI-project FAIRmat to this process will be highlighted, illustrating the importance of defining well-documented metadata catalogues, as well as providing community-specific online data processing capabilities.

MM 22.2 Wed 10:45 H46

A materials informatics framework to discover patterns in atom probe tomography data — ●ALAUKE SAXENA, NIKITA POLIN, BAPTISTE GAULT, CHRISTOPH FREYSOLDT, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf 40237, Germany.

Atom probe tomography (APT) is a unique technique that provides 3D elemental distribution with near-atomic resolution for a given material. However, the large amount of data acquired during the experiment and

the complexity of the 3D microstructures poses a challenge to fully quantify APT data. Here, taking APT measurements corresponding to a Fe-doped Sm-Co alloy as an example, we present an approach based on unsupervised machine learning to extract different phases in the data. On top of this method, we have built a PCA-based workflow to reduce secondary phase precipitates with complex morphology into simpler plate-like morphologies thus enabling the quantification of in-plane compositional and thickness fluctuations, and relative orientations of the precipitates. The labeled data acquired from the PCA-based approach is used to train a U-NET to perform the same task on different APT samples of the same material automatically. The composition and thickness-related insights are expected to help understand the contribution of the particles to the confinement of the magnetic domains of the dominant 2:17 bulk phase, providing further indications to guide the design of future permanent hard magnets.

MM 22.3 Wed 11:00 H46

Correcting density artifacts in Atom Probe reconstructions:

A tip shape-corrected volume reconstruction approach — ●PATRICK STENDER¹, DANIEL BEINKE¹, FELICITAS BÜRGER², and GUIDO SCHMITZ¹ — ¹Institute for Materials Science, University of Stuttgart — ²Fakultät für Mathematik, Universität Regensburg, D-93040 Regensburg, Germany

Atom Probe Tomography enables the chemical investigation of nanometric volumes with single atomic sensitivity in 3D. The tip shape sample is evaporated atom by atom. From the obtained data sequence, the respective volume is reconstructed.

Conventionally, this reconstruction is performed with the assumption of a hemispherical tip apex. This practice can lead to serious volume distortions (local-magnification effect). Instead of using in-situ correlative microscopy to discover the evolution of the tip shape during the measurement, we extract the emitter shape numerically from the event statistics on the 2D detector plane.

The method is based on the fundamental postulate that the detected density of events is linked to the local Gaussian curvature of the tip

apex. Knowing the variation of this curvature, the surface profile is determined by a finite difference scheme. Except for convexity, no further restriction is imposed on the possible tip shapes.

Different simulated and experimental data sets of complex tip shapes will be discussed and compared. The method largely suppresses the local magnification effects appearing at interfaces between materials of contrasting evaporation thresholds.

MM 22.4 Wed 11:15 H46

Neural networks trained on synthetically generated crystals can classify space groups of ICSD powder X-ray diffractograms — ●HENRIK SCHOPMANS^{1,2}, PATRICK REISER^{1,2}, and PASCAL FRIEDERICH^{1,2} — ¹Institute of Theoretical Informatics, KIT, Karlsruhe, Germany — ²Institute of Nanotechnology, KIT, Eggenstein-Leopoldshafen, Germany

Machine learning techniques have successfully been used to extract structural information such as the crystal space group from powder X-ray diffraction (XRD) patterns. However, training directly on simulated patterns from databases like the ICSD is problematic due to its limited size, class-inhomogeneity, and bias toward certain structure prototypes. We propose an alternative approach of generating random crystals with random coordinates by using the symmetry operations of each space group. Based on this approach, we present a high-performance distributed python framework to simultaneously generate structures, simulate patterns, and perform online learning. This allows training on millions of unique patterns per hour. For our chosen task of space group classification, we achieve a test accuracy of 60.4% on new ICSD structure prototypes not included in the statistics dataset guiding the random generation. Instead of space group classification, the developed framework can also be used for other common tasks, e.g. augmentation and mixing of patterns for phase fraction determination. Our results demonstrate, using the domain of X-ray diffraction, how state-of-the-art models trained on large, fully synthetic datasets can be used to guide the analysis of physical experiments.

15 min. break

Topical Talk

MM 22.5 Wed 11:45 H46

Physics guided machine learning tools in analytical transmission electron microscopy — ●CECILE HEBERT^{1,3}, HUI CHEN¹, and ADRIEN TEURTRE^{1,2} — ¹LSME - IPHYS Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — ²Unité Matériaux et Transformations, Université de Lille, France — ³Institut de Matériaux, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Modern transmission electron microscopes are capable of recording large datasets containing both structural and chemical information on a scale ranging from sub-micrometer to atomic resolution. Operated in scanning TEM mode, two kind of chemical information can be obtained: either via energy dispersive X-Ray spectroscopy or via electron energy loss spectroscopy. On modern instruments, both signals can be acquired at the same time. Turning this huge amount of information (datasets can weight up to several Gb) into segmented quantitative information representing the different phases of the specimen is a real challenge. Pure statistical analysis like principal component analysis generally fails because of two main reasons: artifacts linked to the detection chain and/or non uniqueness of a statistical decomposition. The task is generally complicated by the overlap of phases in the specimen thickness and the presence of the same elements in different phases

With the introduction of physical constraints, like a modelling of the spectrum based on prior knowledge, both on the specimen and on the physical process leading to the spectra, it is possible to obtain a physically meaningful spatial segmentation of the data and to proceed with chemical analysis.

MM 22.6 Wed 12:15 H46

Motif Extraction from Crystalline Images in Real Space —

●AMEL SHAMSELDEEN ALI ALHASSAN and BENJAMIN BERKELS — AICES Graduate School, RWTH Aachen University, Germany

Using modern transmission and scanning transmission electron microscopes ([S]TEM), atomic resolution images are readily available. In particular, the amount of data produced is so large that automatic analysis tools are needed.

During the last decade, automatic data analysis methods concerning different aspects of crystal analysis have been developed, for example, unsupervised primitive unit cell extraction and automated crystal distortion and defects detection. However, an automatic, dedicated motif extraction method is still called for by experimentalists. While previous works on motif extraction did good work in, for example, finding the plane symmetries and restoring smeared out features or finding positions in atomic columns, they were either not automated enough, not applicable to atomic scale images, or required special calibration.

Here, we propose and demonstrate a novel method for automatic direct motif extraction from crystalline images based on variational methods. Given an atomic resolution crystalline image, our method employs unit cell extraction to find the atomic structure then solves a minimization problem involving the unit cell projection operator to find the motif. The method was tested on various synthetic and experimental data sets. The results are a representation of the motif in form of an image, primitive unit cell vectors and a denoised reconstruction of the input image.

MM 22.7 Wed 12:30 H46

Analysis of acoustic emission spectra for structural health monitoring — ●KLAUS LUTTER, VIKTOR FAIRUSCHIN, and THORSTEN UPHUES — Institute for Sensor and Actuator Technology, Coburg, Germany

Today, the analysis of vibration and acoustic emission spectra is routinely used for health monitoring of gears in industrial production. Recent developments of extended IIoT networks provide even fleet comparison and optimization of required field service.

Here, we present an extended approach to utilize acoustic emission spectra to monitor the structural health of machining tools like mills or drills to extract degradation and lifetime information from the acoustic emission. A successful application of a spectral analysis will provide a huge impact on production quality as well as tool quality according to different production parameters which are transferred into related spectral properties. Furthermore we follow an experimental approach using contact microphones. Our diagnostic approach is a detailed analysis of the corresponding frequency spectra and in particular the existing harmonic frequencies during milling processes.

We demonstrate the classification of different process parameter sets according to different dominant frequencies via classification algorithms. The retrieved classes of spectra are used for a classical regression model assisted by neural networks to analyse characteristics changes over time. From an industrial perspective this type of analysis is a non-invasive and versatile approach and easily implementable, even in existing production machinery.

MM 22.8 Wed 12:45 H46

Optimizing laser powder bed fusion by machine learning methods — ●DMITRY CHERNYAVSKY — IFW Dresden, Germany

Additive manufacturing (AM) is a revolutionary manufacturing technique, providing design freedom and environmental advantages. Each newly AM processed material usually requires the identification of the optimal parameter set, a cost and time-consuming process, mostly conducted by trial and error. Here we discuss a machine learning approach for AM process parameter optimization on an example of a Zr-based alloy.

MM 23: Computational Materials Modelling: Magnetic & Electrical Properties

Time: Wednesday 15:45–18:30

Location: H44

MM 23.1 Wed 15:45 H44

Electronic structure of the non-centrosymmetric antiferromagnetic delafossite AgCrSe_2 — ●SEO-JIN KIM¹, HAIJING ZHANG¹, MARCUS SCHMIDT¹, MICHAEL BAENITZ¹, GESA SIEMANN², CHIARA BIGI², PHIL D. C. KING², and HELGE ROSNER¹ — ¹Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — ²School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We present the theoretical studies of the electronic structure and the anomalous Hall effect in AgCrSe_2 based on density functional theory together with experimental results. AgCrSe_2 is a layered triangular lattice system that lacks inversion symmetry, and exhibits a ferromagnetic coupling in layer and an antiferromagnetic coupling between Cr adjacent layers. The comparison of the Cr partial DOS determined from the photoemission measurements and the magnetic LDA+U calculations with a value of $U = 0.75$ eV shows a good agreement, revealing that this compound is weakly correlated due to a strong hybridization with the ligands. The Se 4p states are dominating near the Fermi energy, resulting the sizable band split of the order of 300 meV induced by the SOC. Our recent work demonstrates that this system shows an unconventional anomalous Hall effect driven by the Rashba-like spin-orbit coupling due to the non-centrosymmetric structure. The anomalous Hall conductivity was calculated based on the Berry curvature using an effective tight-binding model constructed by the Wannier function approach. The calculated σ_{xy} shows a good agreement to the experimental measurement.

MM 23.2 Wed 16:00 H44

Atomistic simulations of electrocaloric effects in ferroelectric-paraelectric superlattices — ●DIANA ELISA MURILLO NAVARRO^{1,2}, HUGO IMANOL ARAMBERRI DEL VIGO¹, and JORGE ÍÑIGUEZ^{1,2} — ¹Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Luxembourg — ²Department of Physics and Materials Science, University of Luxembourg

Electrocaloric effects (i.e., the temperature change caused by the application or removal of an electric field) in ferroelectric materials could provide us with an alternative to current polluting cooling technologies. Ferroelectric/paraelectric superlattices, such as the $\text{PbTiO}_3/\text{SrTiO}_3$ system, usually present partly-disordered phases of high entropy (e.g., the so-called domain liquid state) whose polarization can be condensed (frozen) under the application of an electric field, potentially triggering a large change in temperature. Here we present our latest theoretical results on such electrocaloric effects obtained from second principles simulations².

Work funded by the Luxembourg National Research Fund through project C18/MS/12705883 *REFOX*.

1 P. Zubko et al., Nature 534, 524 (2016).

2 J.C. Wojdel et al., J. Phys.: Condens. Matt. 25, 305401 (2013).

MM 23.3 Wed 16:15 H44

Magnetically-textured superconductivity in elemental Rhenium — GABOR CSIRE¹, JAMES F ANNETT², ●JORGE QUINTANILLA³, and BALAZS ÚJFALUSSY⁴ — ¹ICN2, Barcelona, Spain — ²University of Bristol, Bristol, United Kingdom — ³University of Kent, Canterbury, United Kingdom — ⁴Wigner Research Centre for Physics, Budapest, Hungary

Recent μSR measurements revealed remarkable signatures of spontaneous magnetism coexisting with superconductivity in elemental rhenium. Here we provide a quantitative theory that uncovers the nature of the superconducting instability by incorporating every details of the electronic structure together with spin-orbit coupling and multi-orbital physics. We show that conventional s-wave superconductivity combined with strong spin-orbit coupling is inducing even-parity odd-orbital spin triplet Cooper pairs, and in presence of a screw axis Cooper pairs* migration between the induced equal-spin triplet component leads to an exotic magnetic state.

MM 23.4 Wed 16:30 H44

Magnetic bond-order potential for iron-cobalt alloys — ●ALEKSEI EGOROV, APARNA SUBRAMANYAM, RALF DRAUTZ, and THOMAS HAMMERSCHMIDT — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

We present a general-purpose analytic bond-order potential for large-scale simulations of magnetic FeCo alloys. The model is based on a d -valent orthogonal tight-binding Hamiltonian in two-center approximation and an embedding term to account for the s electrons. The BOP is a physical model and therefore requires only a comparably small set of reference data and only a small number of parameters to be optimized. It still provides good transferability to properties of FeCo that we did not include in the fit. We demonstrate the transferability of the FeCo BOP for defect formation energies, vibrational properties, and elastic constants. Due to the explicit treatment of magnetism, our BOP can reproduce the main features of the electronic structure of magnetic and nonmagnetic phases. The predictive power of the FeCo BOP yields a reasonable estimate of the order-disorder transition temperature of magnetic B2-FeCo. Our FeCo BOP also reproduces the dense sequence of stable structures for Fe-rich FeCo compounds.

MM 23.5 Wed 16:45 H44

Ab-initio High-Throughput Screening for Magnetic MAX Phases — ●ALI MUHAMMAD MALIK, JOCHEN ROHRER, and KARSTEN ALBE — Materials Modelling, Technical University of Darmstadt, Germany

MAX phases are layered ternary transition metal carbides and nitrides that combine both metallic and ceramic properties such as high toughness and strength at elevated temperatures. So far about ~ 80 single-M containing MAX phases have been synthesised. But very few of these phases, have long-range magnetic order and are mostly based on Cr and/or Mn. It is expected that magnetically ordered MAX phases will be promising in spintronics and magnetocaloric applications. In this work, we systematically search for stable MAX phases with a focus on magnetic properties, by screening about 1200 potential compositions. The thermodynamic stability is based on relative formation enthalpy compared to known competing phases that are present in M-A-X ternary phase diagram obtained from online databases e.g. Materials Project. Based on the evaluation of relative formation enthalpy, we have predicted around ~ 170 new MAX phases that are potentially synthesisable. However, out of these predicted phases, only 2 in total, based on Cr or Mn, were found to have long-range magnetic order. Finally, it is concluded that the incorporation of a late-transition metal into the MAX structure by alloying or unconventional post-synthesis routes, is the way forward for achieving magnetic long-range order.

15 min. break

MM 23.6 Wed 17:15 H44

Energetic and electronic properties of CsK_2Sb surface facets: An *ab initio* study — ●RICHARD SCHIER^{1,2}, HOLGER-DIETRICH SASSNICK², and CATERINA COCCHI^{2,1} — ¹Humboldt-Universität zu Berlin and IRIS Adlershof — ²Carl von Ossietzky Universität Oldenburg

For the efficient generation of ultra-bright electron beams, the microscopic understanding of the electronic structure of the photoemitting materials is crucial. Ternary alkali antimonides have been proposed as a promising class of photocathodes [1-4]. However, still little is known about their surface properties. We fill this gap with an *ab initio* study of the energetic and electronic properties of 7 CsK_2Sb surface facets of low Miller index. We investigate formation energies as a function of chemical potential to quantify the stability of these systems at varying concentration of the atomic species. We find that the (111)-surfaces terminated with K on top of Sb are generally the most stable, except for very high (low) concentrations of Cs (K). Calculated values for the work functions range from 2.33 eV for (100)-surfaces to 3.50 eV for (111)-surfaces terminated with a Sb layer. From the analysis of the band structures we find 4 out of 7 surfaces to be semiconducting. Metallic surfaces are formed upon an excess of metal atoms at the interface with vacuum.

[1] Schmeißer et al., PRAB 21, 113401 (2018). [2] Cocchi et al., JPCM 31, 014002 (2019). [3] Cocchi et al., Sci. Rep. 9, 18276 (2019). [4] Amador & Cocchi, JPCM 33, 365502 (2021).

MM 23.7 Wed 17:30 H44

Modeling Temperature-Dependent Electronic Structure of Semiconductors with a Dynamic Tight-Binding Approach —

•MARTIN SCHWADE, MAXIMILIAN SCHILCHER, and DAVID EGGER — Department of Physics, Technical University of Munich, Garching, Germany

For theoretical calculations of large-scale system sizes or longer time-scale phenomena the computational costs of typical density functional theory can present a steep barrier, which needs to be tackled by development of alternative approaches. Here, we propose an extension of the tight-binding (TB) formalism which allows for the calculation of macroscopic and temperature-dependent properties of semiconductors with little computational effort. In contrast to previous formulations, we fit TB parameters to first-principles energy eigenvalues using machine learning techniques. Furthermore, our TB approach employs hybrid orbital basis functions and addresses the problem of distance-dependent matrix elements by numerical integration of these orbitals. With this, we can maintain the average symmetry of the system as best as possible but still account for dynamic changes to that symmetry, e.g., by lattice distortions and other thermal effects. Our method is particularly helpful for getting an accurate solution of the electronic-structure problem for semiconductors at finite temperatures.

MM 23.8 Wed 17:45 H44

Coupled electronic and lattice degrees of freedom in excitonic insulator candidate Ta₂NiSe₅ and Ta₂NiS₅ — •BANHI CHATTERJEE, JERNEJ MRAVLJE, and DENIS GOLEŽ — Jozef Stefan Institute, Jamova 39, SI 1000, Ljubljana, Slovenia

The origin of phase-transition from a high temperature orthorhombic phase to a low temperature monoclinic phase in Ta₂NiSe₅ is debatable. There are two competing scenarios, namely, a structural instability with a B_{2g} zone center optical phonon and electronic order parameter of excitonic nature breaking the discrete set of lattice symmetries [1-3]. We defined a theoretical description which takes both scenarios on equal footings based on realistic modeling using DFT as a starting point and describe electronic and lattice correlation on a Hartree Fock level. We have identified both excitonic instability and the B_{2g} phonon mode in our calculations and investigate the effect of electron-phonon coupling. Within our methods we have further identified spectroscopic signatures showing the lack of excitonic ordering in the auxiliary compound Ta₂NiS₅ which is in agreement with the experimental ARPES observations [4].

[1] A. Subedi, Phys. Rev. Mater. 4, 083601 (2020). [2] L. Windgätter, M. Rösner, G. Mazza, H. Hübener, A. Georges, A. J. Millis, S. Latini, and A. Rubio, Angel,npj Comp. Mat 7, 14 (2021) [3] G. Mazza, M. Rösner, L. Windgätter, S. Latini, H. Hübener, A.J. Millis, A. Rubio, and A. Georges, Phys. Rev. Lett. 124, 197601 (2020) [4] K. Mu, H. Chen, Y. Li, Y. Zhang, P. Wang, B. Zhang, Y. Liu, G. Zhang, Li. Song, and Z. Sun, J.of Mat. Chem. C. 6, 3981 (2018)

MM 23.9 Wed 18:00 H44

Supermetal-insulator transition in a non-Hermitian network model — •HUI LIU¹, JIHH-SHIH YOU², SHINSEI RYU³, and ION COSMA FULGA¹ — ¹IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstrasse 20, 01069 Dresden, Germany — ²Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan — ³Department of Physics, Princeton University, Princeton, New Jersey, 08540, USA

We study a non-Hermitian and non-unitary version of the two-dimensional Chalker-Coddington network model with balanced gain and loss. This model belongs to the class D[†] with particle-hole symmetry† and hosts both the non-Hermitian skin effect as well as exceptional points. By calculating its two-terminal transmission, we find a novel contact effect induced by the skin effect, which results in a non-quantized transmission for chiral edge states. In addition, the model exhibits an insulator to "supermetal" transition, across which the transmission changes from exponentially decaying with system size to exponentially growing with system size. In the clean system, the critical point separating insulator from supermetal is characterized by a non-Hermitian Dirac point that produces a quantized critical transmission of 4, instead of the value of 1 expected in Hermitian systems. This change in critical transmission is a consequence of the balanced gain and loss. When adding disorder to the system, we find a critical exponent for the divergence of the localization length $\nu = 1$, which is the same as that characterizing the universality class of two-dimensional Hermitian systems in class D.

MM 23.10 Wed 18:15 H44

Dynamical mean-field theory on the high-temperature superconductivity for cerium hydrides under extreme pressure — •YAO WEI and CEDRIC WEBER — King's College London, London, UK

Hydrogen-rich superhydrides are promising high-T_csuperconductors, with superconductivity experimentally observed near room temperature, as shown in recently discovered lanthanide superhydrides at very high pressures, e.g. LaH₁₀ at 170 GPa and CeH₉ at 150 GPa. Superconductivity is believed to be closely related with the high vibrational modes of the bound hydrogen ions. Here we study the limit of extreme pressures (from 200 to 500 GPa or higher) where lanthanide hydrides with large hydrogen content have been observed. We focus on CeH₁₀, the prototype candidate for achieving a large electronic contribution from hydrogen in the electron-phonon coupling. In this work, we use a first-principles calculation platform with the inclusion of many-body corrections to evaluate the detailed physical properties of the Ce-H system and to understand the structure, stability and superconductivity of these systems at ultra-high pressure. We provide a DMFT approach to further investigate conventional superconductivity in hydrogen rich superhydrides.

MM 24: Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 4

Crystal structures

Time: Wednesday 15:45–18:30

Location: H45

Topical Talk

MM 24.1 Wed 15:45 H45

Electromigration effects on the atomic ordering process in hard magnetic L₁₀ intermetallic phases — •DANIEL URBAN^{1,2} and CHRISTIAN ELSÄSSER^{1,2} — ¹Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg — ²Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg

High-performance permanent magnets are needed for many applications in energy and information technology. The L₁₀ phase of FeNi is a promising candidate for a sustainable material that is free of rare-earth elements. However, on earth FeNi can only be found in the disordered A1 crystal structure, although the layered L₁₀ structure is lower in energy. By contrast, the latter was found in meteorites, proving the astronomical long timescales required for the dynamical ordering of the material.

We investigate the atomic migration processes in binary intermetallic L₁₀ phases within the framework of density functional theory. Our main objectives are (i) to develop a thorough understanding of the possibilities to enhance the thermally activated diffusion processes at the atomic scale by electric fields and currents and (ii) an assessment in how far electromigration effects can be effective in processing hard

magnetic materials. We extend the scope to the hard magnetic L₁₀ phases of FePt, FePd, MnAl and MnGa as well as ternary Fe(Pt,Ni). These alloys cover a wide range of thermal ordering time scales and related experimental feasibilities.

MM 24.2 Wed 16:15 H45

Deriving Macroscopic Diffusivity from a Microscopic Master Equation Approach — •DANIEL PFALZGRAF^{1,2}, DANIEL URBAN^{1,2}, and CHRISTIAN ELSÄSSER^{1,2} — ¹Freiburg Materials Research Center (FMF), University of Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg, Germany — ²Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

We present our generalisation of a model formalism that allows the derivation of macroscopic diffusion properties of a crystalline material from jump rates of individual atoms or ions. This work is based on a mathematical formalism modelling the uncorrelated motion of particles on a lattice by a Markov chain, from which a master equation in time and space is constructed. This approach is discussed, reformulated, and generalised to be applicable to any three-dimensional crystal system. Specifically, it is capable of describing the diffusion and drift

of particles in a tilted potential landscape, as e.g. induced by electric fields. We sketch multiple use cases for systems involving point defects and grain boundaries and use the derived framework to discuss the diffusion of oxygen vacancies in strontium titanate.

MM 24.3 Wed 16:30 H45

Atomistic calculations of charged point defects at grain boundaries in SrTiO₃ — ●CONG TAO¹, DANIEL MUTTER¹, DANIEL URBAN¹, and CHRISTIAN ELSÄSSER^{1,2} — ¹Fraunhofer IWM, Freiburg, Germany — ²University of Freiburg, FMF, Germany

Oxygen vacancies have been identified to play an important role in accelerating grain growth in polycrystalline perovskite-oxide ceramics. To advance the fundamental understanding of growth mechanisms at the atomic scale, we performed classical atomistic simulations to investigate the atomistic structures and oxygen vacancy formation energies at grain boundaries in the prototypical perovskite-oxide material SrTiO₃ [1]. We focus on two symmetric tilt grain boundaries, namely $\Sigma 5(310)[001]$ and $\Sigma 5(210)[001]$. Electrostatic potentials are present in supercells containing alternatingly charged lattice planes and grain boundaries. We derive analytic solutions for these potentials for both open and periodic boundary conditions and apply them to our atomistic model structures. In this way, simulation artifacts resulting from the interaction of the electrostatic potential with charged point defects can be corrected, leading to physically reasonable defect energies. We report calculated formation energies of oxygen vacancies on all possible sites across boundaries between the two misoriented grains, and we analyze the values with respect to local charge densities at the vacant sites. The developed calculation procedure can be transferred to more complicated interfaces such as asymmetric tilt grain boundaries [2].

[1] C. Tao, et. al., Phys. Rev. B 104, 054114 (2021).

[2] C. Tao, et. al., arxiv.org/abs/2110.02118.

MM 24.4 Wed 16:45 H45

Field assisted sintering of piezoelectric-bioactive scaffolds for bone tissue engineering — ●ABDULLAH RIAZ¹, CHRISTIAN POLLEY¹, EBERHARD BURKEL², and HERMANN SEITZ¹ — ¹Chair of Microfluidics, Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Rostock, Germany — ²Institute of Physics, University of Rostock, Rostock, Germany

The treatment of critical size bone defects is still a challenge. The external material is often needed to support bone and guide tissue regeneration by physical stimulation. Promising effects of electrical stimulation on bone cell growth have led to an interest in using piezoelectric ceramics for tissue repair. Nevertheless, it is still concerning due to the toxicity of ceramics, which exhibit ion dissolution in biological fluids. In this study, nanostructured pure and doped calcium titanate is prepared by sol-gel synthesis and field assisted sintering. The piezoelectric behaviour is observed in calcium titanate, which is also a non-cytotoxic compound. This behaviour is referred to as pseudo-piezoelectricity since it is generated by the distorted structure which is formed during densification by field assisted sintering. Additionally, piezoelectric barium titanate-45S5 bioactive glass composites are combined with titanium alloy Ti6Al4V for the potential implantation of piezoelectric-bioactive scaffolds in load-bearing areas. For the engineering of these bulk scaffolds, electron beam melting is utilized for manufacturing metallic load-bearing lattice structures and combined with piezoelectric-bioactive composites for the joint processing via field assisted sintering.

15 min. break

MM 24.5 Wed 17:15 H45

Microstructure and hardness of self-passivating SMART alloys manufactured via field assisted sintering technology — ●JIE CHEN¹, ANDREY LITNOVSKY¹, XIAOYUE TAN², and CHRISTIAN LINSMEIER¹ — ¹Forschungszentrum Jülich GmbH, IEK-4, 52425 Jülich, Germany — ²School of Materials Science and Engineering, Hefei University of Technology, 230009 Hefei, China

Self-passivating Metal Alloys with Reduced Thermo-oxidation

(SMART) with a composition of W-11.4wt%Cr-0.6Y% is a promising candidate for plasma facing material of a future fusion power plant. In addition to sputtering resistance under plasma exposure, the laboratory-made bulk SMART system has exhibited excellent anti-oxidation performance at 1273K in humid environment relevant to accident conditions. The field assisted sintering technology is applied to manufacture SMART alloy. The microstructure of SMART alloy is intimately related to production parameters including heating ramp, sintering temperature, thermal holding time and applied pressure. Heating rate and appropriate sintering temperature are considered important to obtain ultrafine or nanosized grain. The machinability of sintered SMART alloy is under investigation in which hardness and thermal conductivity are of particular interest. The as-sintered SMART alloy with 1217 HV0.5 is obtained by heating at a rate of 200K/min to 1460°C and applying pressure of 50 MPa. There is an attempt to reduce the material's hardness to facilitate its application in fusion reactor. Details of the work are presented in the contribution.

Topical Talk

MM 24.6 Wed 17:30 H45

From Uncovering the Mechanisms of Flash Sintering to Realizing Ultrafast Sintering without Electric Fields and Discovering Electrochemically Driven Microstructural Evolution — ●JIAN LUO — University of California San Diego, U.S.A.

This talk will first review our recent studies on understanding the scientific questions and technological opportunities of flash sintering [Scripta 146: 260 (2018); MRS Bulletin 46: 26 (2021)]. We originally proposed that flash sintering generally starts a thermal runaway [Acta 94:87 (2015)], but it can also be activated by bulk phase and grain boundary complexion transitions [Acta 181:544 (2019)]. We further proved that ultrafast densification is enabled by ultrahigh heating rates of ~ 100 K/s [Acta 125:465 (2017)]. Subsequently, a generic ultrafast high-temperature sintering was reported in a collaborative study [Science 368:521 (2020)]. Other related technologies include water-assisted flash sintering (WAFS) to flash ZnO at room temperature [Scripta 142:79 (2018)] and two-step flash sintering (TSFS) to densify ceramics with suppressed grain growth [Scripta 141:6 (2017)]. Recent research discovered electrochemically induced grain boundary transitions that can cause enhanced or abnormal grain growth [Nature Communications 12:2374 (2021)]. Subsequently, I will discuss a series of on-going studies to further investigate electrochemically controlled microstructural evolution and tailor the microstructural evolution with applied electric fields in various systems and schemes [Yan et al., unpublished work].

Topical Talk

MM 24.7 Wed 18:00 H45

Electric fields effects in ionic conductors during flash sintering and ion exchange — ●MATTIA BIESUZ, GIAN DOMENICO SORARU, and VINCENZO MARIA SGLAVO — University of Trento, Trento, Italy

Electric fields can drive ceramic ionic conductors out of the equilibrium dictated by temperature, composition, and pressure. These phenomena can be used to promote ceramics sintering or ion exchange.

Herein, we explore flash sintering in oxygen ionic conductors (YSZ and GDC) evidencing the presence of some electrochemical effects producing alterations of the defect chemistry and activating n-type electronic conductivity. This enhances the conductivity of the green sample, increases the electric power dissipation and contributes to the activation of the flash leading to sudden densification of ceramics. The pivotal role of electrochemical reduction during DC-flash sintering impacts the thermal history of the flashed samples generating strong thermal gradients between the cathode and anode which can be enhanced or removed by changing the quality and type of the used electrodes. The electrochemical description of flash sintering in oxygen ion conductors well explains the electrode configuration and atmosphere effects on the flash processes.

Electrochemical phenomena are, however, pivotal also in other ionic conductor systems subjected to flash-like processes. It is shown that the electrode material choice strongly affects the flash behavior and modifies the glass composition in the vicinity of electrodes. Hence, electric fields can be to modify the surface glass or ceramics composition improving mechanical and functional properties.

MM 25: Data Driven Materials Science: Computational Frameworks / Chemical Complexity

Time: Wednesday 15:45–18:30

Location: H46

Topical Talk

MM 25.1 Wed 15:45 H46

Automated atomistic calculation of thermodynamic and thermophysical data — ●JAN JANSSEN^{1,2}, TILMANN HICKEL^{1,3}, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — ²Los Alamos National Laboratory, Los Alamos, USA — ³Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, 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 - <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.

MM 25.2 Wed 16:15 H46

Efficient parameterization of the atomic cluster expansion — ●ANTON BOCHKAREV, YURY LYSOGORSKIY, MATOUS MROVEC, and RALF DRAUTZ — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

The atomic cluster expansion (ACE) is a machine learning model with a complete basis set representation that can be used for constructing interatomic potentials. These potentials can be both, general-purpose as well as potentials designed for a specific application. The former are usually more reliable and accurately describe materials in various conditions, but building such models often requires a materials specific expertise and extensive training datasets. Purpose-specific potentials have only limited ranges of applicability, but are also less demanding in terms of training data. Here we demonstrate a complete, efficient and largely automated framework for constructing quantum accurate ACE models for various applications. Our framework includes automated data generation, model parameterization and validation. Efficient implementations on CPU and GPU hardware enable large scale simulations.

MM 25.3 Wed 16:30 H46

Atomic cluster expansion for Mg: From defects to phase diagrams — ●ESLAM IBRAHIM, YURY LYSOGORSKIY, MATOUS MROVEC, and RALF DRAUTZ — ICAMS, Ruhr Universität Bochum, 44780 Bochum, Germany

In this work, we developed a general-purpose parametrization of the atomic cluster expansion (ACE) for Mg. The model shows an outstanding transferability over a broad range of atomic environments and is able to capture physical properties of bulk as well as defective Mg phases in excellent agreement with reference first-principles calculations. We demonstrate the computational efficiency and the predictive power of ACE by calculating the phase diagram covering temperatures up to 3000 K and pressures up to 80 GPa using state-of-the-art thermodynamic integration techniques implemented in the CALPHY software package. The ACE predictions are compared with those of common interatomic potentials, such as the embedded atom method or the angular-dependent potential, as well as a recently developed neural network potential. The comparison reveals that ACE is the only model that is able to predict both qualitatively and quantitatively correctly the phase diagram in close agreement with experimental observations.

MM 25.4 Wed 16:45 H46

Learning design rules for selective oxidation catalysts from high-throughput experimentation and artificial intelligence — ●LUCAS FOPPA¹, CHRISTOPHER SUTTON¹, LUCA M. GHIRINGHELLI¹,

SANDIP DE², PATRICIA LÖSER³, STEPHAN SCHUNK^{2,3}, ANSGAR SCHÄFER², and MATTHIAS SCHEFFLER¹ — ¹The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Germany — ²BASF SE, Germany — ³hite GmbH, Germany

The design of heterogeneous catalysts is challenged by the complexity of materials and processes that govern reactivity and by the very small number of good catalysts. Here, we show how the subgroup-discovery (SGD) artificial-intelligence *local* approach[1] can be applied to an experimental plus theoretical data set to identify constraints or *rules* on key physicochemical parameters that exclusively describe materials and reaction conditions with outstanding catalytic performance.[2] By using high-throughput experimentation, 120 SiO₂-supported catalysts containing Ru, W and P were synthesized and tested in propylene oxidation. As candidate descriptive parameters, the temperature and ten calculated parameters related to the composition and chemical nature of elements in the catalyst materials, were offered. The temperature, the P content, and the composition-weighted electronegativity are identified as key parameters describing high yields of value-added oxygenate products. The SG rules reflect the underlying processes associated to high performance, and guide catalyst design.

[1] B.R. Goldsmith, *et al.*, *New. J. Phys.* **19**, 013031 (2017).[2] L. Foppa, *et al.*, *ACS Catal.* **12**, 2223 (2022).**15 min. break****Topical Talk**

MM 25.5 Wed 17:15 H46

Understanding Dislocation Flow and Avalanches in High Entropy Alloys by Machine Learning-based Data Mining of In-Situ TEM Experiments — ●STEFAN SANDFELD — FZJ/IAS-9, 52068 Aachen, Dennewartsstr. 25-27

This talk will give an overview over recent developments in the field of material informatics and materials data science, in particular over current, state-of-the-art machine learning and data-mining techniques in the context of TEM experiments.

As a main example, the goal is to understand some of the many open questions concerning the underlying structure-property relations in High Entropy Alloys (HEAs). Although in-situ Transmission Electron Microscopy (TEM) allows high-resolution studies of the structure and dynamics of moving dislocations and – in a way – makes the local obstacle/energy "landscape" visible through the geometry of dislocations; a 3D analysis and high-throughput data-mining of the resulting data is still not possible.

We introduce a novel data-mining approach that is based on spatio-temporal coarse graining of TEM dislocation data, making ensemble averaging of a large number of snapshots in time possible. Using dislocations as "probes" we investigate the effect of pinning points on the dislocation glide behavior of CoCrFeMnNi alloy during in-situ TEM straining. Additionally, we use our Deep Learning-based dislocation extraction and 3D reconstruction to analyze the strain avalanche statistics of in-situ TEM recordings and discuss the dependency of the power law exponent based on 3D dislocation dynamics simulations.

MM 25.6 Wed 17:45 H46

Phase stability and short range order in CrCoNi medium entropy alloy — ●SHEULY GHOSH¹, VADIM SOTSKOV², ALEXANDER SHAPEEV², FRITZ KOERMANN^{1,3}, and JOERG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH — ²Skolkovo Institute of Science and Technology — ³Delft University of Technology

One of the key components in the design and exploration of multi-component alloys is the knowledge about its phase stability. The solid solution of multicomponent alloys are often assumed to be ideally random. However, short-range order, which is challenging to quantify by experiments, is known to affect the mechanical properties of alloys. An important issue to address is therefore to quantify the degree of local chemical ordering as function of temperature and its chemical nature.

In the present work, we have investigated short-range order (SRO) and its impact on phase stability in CrCoNi medium entropy alloy. This alloy is known for its cryogenic damage tolerance and general mechanical superiority. For this purpose, we have employed a recently proposed computationally efficient on-lattice machine-learning interatomic potential called low-rank potentials. These potentials are capable of accurately representing interactions in a system with many

chemical components which is used in subsequent Monte Carlo simulations. The potentials are trained on DFT supercell calculations and thus allow to systematically include the impact of local lattice distortions. The computed short-range order parameters and observed ordering are discussed in view of recent simulation and experimental works.

MM 25.7 Wed 18:00 H46

Inverse Design of Multicomponent Crystalline Materials — TENG LONG^{1,2} and HONGBIN ZHANG¹ — ¹Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany — ²School of Materials Science and Engineering, Shandong University, Jinan 250061, China

Autonomous materials discovery with desired properties is one of the ultimate goals of materials science. In this work, we implement and apply constrained crystal deep convolutional generative adversarial networks to design unreported (meta-)stable crystal structures. The essential continuous latent space is obtained based on the voxel construction of crystal structures, resulting in an image-based latent space which is proven to be a robust descriptor for forward inference of various physical properties. This also allows prediction of new crystal structures based on generative adversarial network. Furthermore, taking the formation energy as an example, it is demonstrated how the physical properties can be optimized automatically in the latent space while exploring a big chemical space to predict novel phases. Such an approach has been successfully applied on binary (e.g., Bi-Se) and

multicomponent systems, which paves the way to achieve the inverse design of crystalline materials via multi-objective optimization.

MM 25.8 Wed 18:15 H46

Databases for Machine Learning of Grain Boundary Segregation — ALEXANDER REICHMANN¹, CHRISTOPH DÖSINGER¹, DANIEL SCHEIBER², OLEG PEIL², VSEVOLOD RAZUMOVSKIY², and LORENZ ROMANER¹ — ¹Department of Materials Science, Leoben, Austria — ²Materials Center Leoben Forschung GmbH, Leoben, Austria

The chemical and structural state of grain boundaries (GBs) is of great importance for the design and performance of many technologically relevant materials. On the basis of atomistic simulations, the relevant quantities of GB, in particular the segregation energy has been calculated for many materials. On the experimental side, the concentration of solute elements at the GBs can be measured with a variety of techniques including in particular Auger spectroscopy or Atom Probe Tomography. When comparing calculated segregation energies with segregation energy gained from experimental excess data, good agreement is not always observed. In this talk we will present our current and planned activities regarding creation of segregation databases and application of data driven models. One of these is the Bayesian inference framework, which we used in combination with Markov chain Monte Carlo simulations for uncertainty quantification and model evaluation. These activities shall lead to a better understanding of the deviation between DFT-calculated and experimentally determined GB excess.

MM 26: Members' Assembly

Time: Wednesday 18:45–20:15

Location: H44

All members of the Metal and Material Physics Division are invited to participate.

MM 27: Invited Talk Christian Greiner

Time: Thursday 9:30–10:00

Location: H44

Invited Talk MM 27.1 Thu 9:30 H44
Crystal rotation kinematics during the tribological loading of high-purity copper — CHRISTIAN GREINER — Karlsruher Institut für Technologie (KIT), Kaiserstrasse 12, 76131 Karlsruhe

Friction, wear and the associated energy dissipation are major challenges from nanoelectromechanical systems, over hip implants to offshore wind turbines. Already in 1950, Bowden and Tabor pointed out that in metallic tribological contacts the majority of the dissipated energy is spent 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. One key process involved therein is the re-orientation of the crystal lattice, or crystal rotation, due to the shear load imposed by the sliding contact. Our work sheds light on the early stage, fundamental mechanisms of tribologically induced lattice rotation kinematics. Using a high-purity copper bicrystal and a sapphire sphere, unlubricated, single-pass sliding tests were conducted. Electron backscatter diffraction (EBSD) performed directly on the wear track reveals a crystal rotation process around the transverse direction at the heart of tribologically induced lattice rotation, irrespective of sliding direction, grain orientation and normal load. A detailed analysis corroborates that surprisingly, changing the sliding direction merely alters the precise accommodation of crystal rotations, but not their fundamental nature.

MM 28: Transport in Materials: Diffusion / Electrical Transport & Magnetism

Time: Thursday 10:15–11:30

Location: H44

MM 28.1 Thu 10:15 H44
Electrical resistivity of magnetron-sputtered Fe_{1-x}O thin films — SIMON EVERTZ¹, NINA NICOLIN¹, DANIEL PRIMETZHOFFER², JAMES P. BEST¹, and GERHARD DEHM¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — ²Department of Physics and Astronomy, Uppsala University, S-75120 Uppsala, Sweden

Fe_{1-x}O (wüstite) is a critical phase for a number of applications in the future hydrogen economy, such as photochemical materials for H₂ production by water-splitting. Hence, charge transport is crucial for the applicability of Fe_{1-x}O in electrode materials. To probe the charge transport of close-to-stoichiometric Fe_{1-x}O, thin films were synthesized by reactive magnetron sputtering with systematically varied O₂ gas flow. The phase formation and chemical composition was correlated to the electrical resistivity and mechanical properties, as measured in a van-der-Pauw-setup and nanoindentation, respectively. The

charge transport mechanism is shown to change from thermally activated hopping of charge carriers - typical for a semiconductor - to metallic-like behavior as a function of the phase purity of the films. By correlative analysis of phase purity, microstructure and mechanical properties, it is shown that already small amounts of Fe as impurity phase are decisive for changing the charge transport mechanism. These significant changes in charge transport are further compared to the hardness and Young's modulus of these films.

MM 28.2 Thu 10:30 H44

Electronic structure and transport properties of NdTe₃ — KIRSTINE J DALGAARD¹, SHIMING LEI¹, CLAUDIUS MÜLLER², STEFFEN WIEDMANN², MARTIN BREMHOLM³, and LESLIE M SCHOOP¹ — ¹Department of Chemistry, Princeton University, Princeton, NJ, USA — ²High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, Netherlands — ³Department of Chemistry, Aarhus University, Aarhus, Denmark

The delocalized, hypervalent bonding in some main group element square-net materials have been linked to fascinating phenomena, including band inversions with high charge carrier mobility, and topologically nontrivial band structures. The family of rare earth tritellurides crystallize in a van der Waals structure with double tellurium square-nets, where the tellurium p orbitals form the Fermi energy crossing bands, and the partly filled 4f orbitals give rise to a rich spectrum of magnetic properties. The tellurium square-nets also undergo incommensurate charge density wave transitions affecting the band structure in ways that are yet to be fully understood. In this work, we studied the electronic structure of neodymium tritelluride through quantum oscillation and transport measurements. A remarkably high electron mobility for a magnetic van der Waals material was found, suggesting steeply dispersed bands, along with thus far unreported deviations from conventional Lifshitz-Kosevich behavior.

MM 28.3 Thu 10:45 H44

Non-coplanar magnetism, topological density wave order and emergent symmetry at half-integer filling of moiré Chern bands — ●PATRICK WILHELM¹, THOMAS LANG¹, MATHIAS SCHEURER¹, and ANDREAS LÄUCHLI^{1,2,3} — ¹Institut für Theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria — ²Laboratory for Theoretical and Computational Physics, Paul Scherrer Institute, 5232 Villigen, Switzerland — ³Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We study the impact of Coulomb interactions at half-integer filling of the moiré Chern bands of twisted double-bilayer graphene and twisted mono-bilayer graphene, using unbiased exact diagonalization complemented by unrestricted Hartree-Fock calculations. For small intrasublattice tunneling, wAA, a non-coplanar magnetic state is found which has the same symmetries as the tetrahedral antiferromagnet of the triangular moiré lattice and can be thought of as a skyrmion lattice commensurate with the moiré scale. The antiferromagnetic order competes with a set of ferromagnetic, topological charge density waves, which are favored for larger wAA and are associated with an approximate emergent O(3) symmetry, 'rotating' the different charge density wave states into each other. Exhibiting a finite charge gap and Chern number $C=|1|$, the formation of charge density wave order which is intimately connected to a skyrmion lattice phase is consistent with recent experiments on these systems.

MM 28.4 Thu 11:00 H44

Interference effects in one-dimensional moiré crystals — ●NILS WITTEMEIER¹, MATTHIEU J. VERSTRAETE^{2,4}, PABLO ORDEJÓN¹, and ZEILA ZANOLLI^{3,4} — ¹Catalan Institute of Nanoscience and Nanotechnology, ICN2 (CSIC, BIST), Bellaterra, Spain — ²NanoMat/Q-

Mat/CESAM, Université de Liège (B5), Liège, Belgium — ³Chemistry Department & Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, the Netherlands — ⁴ETSF

This work [1] investigates interference effects in finite sections of 1D moiré crystals using the Landauer-Büttiker formalism within the tight-binding approximation. We explain interlayer transport in double-wall carbon nanotubes and demonstrate that wave function interference is visible at the mesoscale: in the strong coupling regime, as a periodic modulation of quantum conductance and emergent localized states; in the localized-insulating regime, as a suppression of interlayer transport, and oscillations of the density of states. The interlayer transmission between strongly coupled metallic nanotubes is limited to either $1G_0$ or $2G_0$. Our results could be exploited to design quantum electronic devices, e.g. nonelectric switches based on chiral nanotubes. Most importantly, we clarify the origin of the so-far unexplained $1G_0$ quantum conductance measured in multi-wall carbon nanotubes [2, 3].

[1] N. Wittemeier *et al.* Carbon **186**, 416 (2022)

[2] S. Frank *et al.* Science **280** (1998)

[3] W. A. de Heer & C. Berger, Phys. Rev. Lett. **93**, 259701 (2004)

MM 28.5 Thu 11:15 H44

On correlations between local chemistry, distortions and kinetics in high entropy nitrides: an ab initio study — ●DAVID HOLEC¹, GANESH K. NAYAK¹, ANDREAS KRETSCHMER², PAUL H. MAYRHOFER², MARCUS HANS³, and JOCHEN M. SCHNEIDER³ — ¹Department of Materials Science, Montanuniversität Leoben, Leoben, Austria — ²Institute of Materials Science and Technology, TU Wien, Vienna, Austria — ³Materials Chemistry, RWTH Aachen University, Aachen, Germany

High entropy alloys (HEAs) have triggered significant scientific interest due to their unusual structural stability combined with excellent mechanical and other functional properties. Recently, exploration of materials used as protective coatings has also entered this room by exploring high entropy borides, oxides, carbides, and nitrides. These chemically complex systems provide huge combinatorial space for tuning the composition, hence making the experimental exploration tedious. High-throughput simulations based on unbiased ab initio calculations provide an ideal tool to guide the experiments.

We will show that for high entropy nitrides (HENs), strain is equally important for the stabilization as entropy. Our predictions were validated by experimental investigations on the thermal stability of selected HEN coatings. The predicted structures are further characterized in terms of their local distortions, one of the core effects of HEAs. Another core effect is sluggish bulk diffusion. Therefore, in the second part of the talk, we will explore correlations between migration barriers for bulk diffusion, local chemical compositions, and local distortions.

MM 29: Data Driven Materials Science: Design of Functional Materials

Time: Thursday 10:15–11:30

Location: H45

MM 29.1 Thu 10:15 H45

Investigations of the Polysulfide Conversion Mechanism via Gaussian Approximation Potentials — ●XU HAN^{1,2}, CARSTEN G. STAACKE¹, HENDRIK H. HEENEN¹, XUEFEI XU², and KARSTEN REUTER¹ — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²Tsinghua University, Beijing, China

Lithium-sulfur (Li-S) batteries have been regarded as promising energy storage systems with ultra-high theoretical energy density. During a charging cycle Li_2S is converted to S_8 and vice-versa, where intermediate Li polysulfides (LiPS) are formed in a complex reaction mechanism which is still under debate. The theoretical exploration of the involved Li-S chemistry is challenged by an extended reaction network making it intractable for first principles methods. In contrast, machine learning interatomic potentials (MLIPs) which potentially retain predictive accuracy at a fraction of the computational cost are ideally suited for this task.

Here, we establish a training protocol for a Gaussian approximation potential (GAP) to simulate the chemistry of LiPS. Our training is based on a constrained on-the-fly exploration of the LiPS chemical space. In that, we enumerate the connectivity of (poly)cyclic LiPS and explore their stability via global optimization procedures with iteratively refined MLIPs. We use the final, sufficiently accurate MLIP to sample the LiPS phase space and to compute charging/discharging

curves which we can directly compare to experimental data. Our MLIP calculations are expected to provide more fundamental insights into the LiPS conversion mechanism in Li-S batteries.

MM 29.2 Thu 10:30 H45

Accelerating the High-Throughput Search for new Thermal Insulators with Symbolic Regression — ●THOMAS PURCELL¹, MATTHIAS SCHEFFLER^{1,2}, LUCA M. GHIRINGHELLI^{1,2}, and CHRISTIAN CARBOGNO¹ — ¹The NOMAD Laboratory at Fritz-Haber-Institut der Max-Planck-Gesellschaft — ²FAIRmat at Humboldt Universität zu Berlin, Berlin, Germany

Reliable artificial-intelligence models are key to accelerate the discovery of new functional materials for various applications. Here, we present a general, data-driven framework that combines symbolic regression with sensitivity analysis to create hierarchical workflows. We illustrate the power of this new framework by screening for new thermally insulating materials. We first use the sure-independence screening and sparsifying operator (SISSO) [1] to build an analytical model that describes the thermal conductivity of a material and then extract out the most important input properties using a variance-based sensitivity analysis [2]. Using the information gained from the analysis we screen over a set of 732 materials and find the region of space most likely to contain strong thermal insulators. Finally we confirm these

predictions by calculating thermal conductivities using the *ab initio* Green-Kubo technique [3].

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

[2] S. Kucherenko, S. Tarantola, and P. Annoni. *Comput. Phys. Commun.* **183**, 937 (2012)

[3] C. Carbogno, R. Ramprasad, and M. Scheffler. *Phys. Rev. Lett.* **118**, 175901 (2017)

MM 29.3 Thu 10:45 H45

Uncertainty Modelling for Property Prediction of Double Perovskites — ●SIMON TESHUVA¹, MARIO BOLEY¹, FELIX LUONG¹, LUCAS FOPPA², and MATTHIAS SCHEFFLER² — ¹Monash University, Melbourne, Australia — ²Fritz Haber Institute, Berlin, Germany

Statistical predictive models for double perovskite properties are of high interest, because the perovskite structure allows relatively accurate property prediction and at the same time provides enough flexibility to yield a huge number of different materials of which some are likely relevant for important applications. Existing results published for this class of materials typically refer only to the predictive performance as, e.g., measured by the root mean squared error. However, active learning strategies for effective materials screening also rely on adequate uncertainty estimates as provided by probabilistic models.

Here, we study the predictive performance of two popular machine learning models, Gaussian processes and random forests, together with the quality of their uncertainty estimates. This study is based on a dataset of over 800 single (ABO₃) and double (A₂BB'O₆) cubic perovskite oxides with computed bulk modulus, cohesive energy, and bandgap. We show that Gaussian processes, while providing sound Bayesian uncertainty estimates, can have inferior performance when their assumption of isometric smoothness of the target property is not met. In this case, as exemplified by the double perovskite bandgaps, random forests provide a better alternative, despite their rather ad-hoc uncertainty estimates. Improving these estimates thus appears to be a promising direction for future research.

MM 29.4 Thu 11:00 H45

Automated effective Hamiltonian construction and active sampling of potential energy surface by Bayesian optimization — ●MIAN DAI, YIXUAN ZHANG, and HONGBIN ZHANG — Institute of Materials Science, Technical University of Darmstadt, Darmstadt, 64287, Germany

A first-principles effective Hamiltonian method can be used to simulate the phase transition sequences. In practice it is quite tedious to express the total energy surfaces and estimate reasonable parameters for high-order polynomials. We implemented Bayesian optimization (BO) to sample the total energy surfaces based on active learning and fit the set of parameters for constructing the effective Hamiltonians. Taking BaTiO₃ as a case study, we found that less than 30 sampling configurations with automated generated structures by BO are enough to determine a new set of parameters. The hyperparameter in our BO process is tuned to show the improvement of the convergence for all fitted parameters. Using the new set of parameters, we perform Monte Carlo simulations which produce comparable phase transition temperatures with experimental values and previous results. Our BO algorithm has a great potential for future application in construction the effective Hamiltonians with more complicated subspace and effective atomic potentials describing the full lattice dynamics.

MM 29.5 Thu 11:15 H45

Predicting oxidation and spin states by high-dimensional neural networks — ●KNUT NIKOLAS LAUSCH¹, MARCO ECKHOFF¹, PETER BLÖCHL², and JÖRG BEHLER¹ — ¹Georg-August-Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Göttingen, Germany — ²Technische Universität Clausthal, Institut für Theoretische Physik, Clausthal-Zellerfeld, Germany

Machine learning potentials (MLP) such as high-dimensional neural network potentials (HDNNP) provide first-principles quality energies and forces enabling large-scale molecular dynamics simulations at low computational costs. However, most current MLPs do not provide any information about the electronic structure of the system, which is often important for a detailed understanding of complex systems such as transition metal oxides. The lithium intercalation compound Li_xMn₂O₄ (0 ≤ x ≤ 2), a commercially used cathode material in lithium ion batteries, is such a system since the manganese ions adopt different oxidation states based on the lithium content and distribution. Here, we propose a high-dimensional neural network (HDNN) that can predict atomic oxidation and spin states as a function of the local atomic environments in Li_xMn₂O₄. The HDNN can complement HDNNP-driven MD simulations giving insights into the underlying electronic processes that give rise to complex phenomena such as a charge ordering transition, and electrical conductance.

MM 30: Liquid and Amorphous Metals

Time: Thursday 10:15–13:00

Location: H46

MM 30.1 Thu 10:15 H46

Controlling the degree of rejuvenation and strain-hardening in metallic glasses — ●DANIEL ŞOPU^{1,2}, XUDONG YUAN¹, and JÜRGEN ECKERT^{1,3} — ¹Erich Schmid Institute of Materials Science, Leoben, Austria — ²Technische Universität Darmstadt, Germany — ³Montanuniversität Leoben, Austria

The correlation between the degree of rejuvenation and strain-hardening in metallic glasses (MGs) is investigated using molecular dynamics simulations. By randomly removing atoms from the glass matrix, free volume is homogeneously generated and glassy states with different degrees of rejuvenation are designed and further mechanically tested. The highest rejuvenated state is defined by the dynamic balance between free volume generation and annihilation. The highest degree of rejuvenation correlates to the flow strain of the materials and the structure is similar to that found in shear bands. The free volume in the rejuvenated glasses can be annihilated under tensile or compressive deformation that consequently leads to structural relaxation and strain-hardening. Loading-unloading cycling tensile tests are simulated and the atomic-scale mechanism of strain-hardening in the highly rejuvenated MGs is highlighted.

MM 30.2 Thu 10:30 H46

Revealing the impact of Sulfur addition on the medium-range order and relaxation dynamics of metallic glasses — ●HENDRIK VOIGT¹, NICO NEUBER², HARALD RÖSNER¹, MARTIN PETERLECHNER¹, RALF BUSCH², and GERHARD WILDE¹ — ¹Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany — ²Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

The addition of Sulfur as an alloying element has been shown to enable or improve the glass forming ability of certain glasses drastically [1]. Despite growing knowledge of the impact that Sulfur has on the mechanical properties, the underlying structure and its dynamics are still not fully understood [2].

In this contribution the sample system Pd₃₁Ni₄₂S₂₇ has been investigated with respect to medium-range order (MRO). For the MRO analysis multiple series of nanobeam diffraction patterns with varying probe sizes were acquired in order to conduct variable resolution Fluctuation Electron Microscopy (FEM). Furthermore, Electron Correlation Microscopy (ECM) was employed to analyse relaxation dynamics by the acquisition of a tilted dark-field time series. By the combination of these two techniques it appears that the size of the regions displaying strongly decelerated dynamics at room temperature correlate with the detected MRO. The results are discussed with respect to current models.

[1] A. Kuball et al., *Scripta Materialia* (2018) 73-76 [2] H. Jiang et al., *Scripta Materialia* (2021) 116923

MM 30.3 Thu 10:45 H46

Glass Formation and Shear Banding in High-Entropy Metallic Glasses: A Molecular Dynamics Study — ●MARIE J. CHARRIER, DANIEL T. UTT, ARNE J. KLUMP, and KARSTEN ALBE — Fachgebiet Materialmodellierung, Institut fuer Materialwissenschaft, Technische Universitaet Darmstadt

Bulk metallic glasses (BMGs) and High-Entropy Alloys (HEAs) both comprise a large number of elements but deviate strongly in their mechanical properties. BMGs are strong but brittle and usually derived from crystalline binary subsystems with deep eutectics and intermetal-

lic phases. HEAs, on the other hand, show remarkable ductility, a small heat of mixing, and are thus typically not glass formers. The open question is whether a classically crystalline random solid solution HEA can be transformed into a BMG using appropriate processing. In this work, we use atomistic computer simulations to study the combination of the two materials classes, HE-MGs. Here, we are able to kinetically suppress crystallization in the CrMnFeCoNi alloy, which in the real world remains a crystalline single-phase solid solution using conventional quench rates. First, we investigate the thermodynamics of the glass transition and its dependence on quench rate. Second, the phase stability of the HE-MG is compared to the crystalline HEA. Third, the atomic-level structure is characterized in terms of chemical and structural short- and medium-range order. Last, we perform compressive and tensile testing on HE-MG samples to assess failure by homogeneous deformation or shear localization and compare the mechanical properties against a CoCrFeMnNi nanocrystal.

MM 30.4 Thu 11:00 H46

Cyclical structural relaxation of PdNiP and micro-alloyed PdNiPFe and PdNiPCo glasses — ●MANOEL W. DA SILVA PINTO, MARK STRINGE, KATHARINA SPANGENBERG, HARALD RÖSNER, and GERHARD WILDE — Institut für Materialphysik, WWU Münster

Relaxation phenomena in Pd₄₀Ni₄₀P₂₀ bulk metallic glasses (BMG) as well as in micro-alloyed forms of Co and Fe addition were investigated by calorimetry. The BMGs were submitted to different thermal treatments by varying temperatures and times. In order to identify distinct signatures of relaxation, the thermal and temporal evolution of enthalpic contributions to calorimetric signals were analyzed using different kinetic models. A possibility was found to control the formation and depletion of an endothermic signature before the glass transition by quenching and annealing procedures. From the evolution of the enthalpies with annealing time and from isothermal heat flow, time constants related to structural relaxation were obtained and supplemented by dynamical and structural TEM analyses. The obtained results are discussed with respect to existing models for glass relaxation.

MM 30.5 Thu 11:15 H46

Enhancing ductility and strain hardening by modulating residual stresses in metallic glasses — ●XUDONG YUAN¹, DANIEL ŞOPU^{1,2}, and JÜRGEN ECKERT^{1,3} — ¹Erich Schmid Institute of Materials Science, Leoben, Austria — ²Technische Universität Darmstadt, Darmstadt, Germany — ³Montanuniversität Leoben, Leoben, Austria

The correlation between the deformation behavior and the residual stress modulation in metallic glasses (MGs) is investigated using molecular dynamics simulations. Particularly, the influence of residual compressive stress and stress heterogeneity on the tensile deformation behavior of amorphous Cu₆₄Zr₃₆ alloys is investigated. Strain hardening together with enhanced tensile ductility in monolithic MGs can be attained by only modulating the internal stress without changing their local structure. The stress heterogeneity changes the shear band dynamics leading to the formation and interaction of multiple shear bands, which consequently enhances the macroscopic ductility. Additionally, the residual compressive stress offsets the external tensile stress, which delays shear band formation and enables strain hardening in uniaxial tensile tests.

15 min. break

MM 30.6 Thu 11:45 H46

Origin of the Invar effect in Fe-based bulk metallic glasses — ●ALEXANDER FIRLUS¹, MIHAI STOICA¹, STEFAN MICHALIK², ROBIN E SCHÄUBLIN¹, and JÖRG F LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland. ²Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK

Generally, metals, including most ferromagnetic ones, have a constant coefficient of thermal expansion (CTE). However, a few magnetic alloys show an anomalously low CTE below their Curie temperature. At the Curie temperature it increases abruptly by up to one order of magnitude. This effect is known as the Invar effect. While it is rare in crystalline alloys, it is universally observed in ferromagnetic Fe-based bulk metallic glasses (BMGs). To this day, it is still unclear in which way the amorphous atomic arrangement creates the Invar effect and how it manifests at the atomic scale.

In this work we studied BMGs with only one magnetic atom species,

Fe, by in-situ high-energy X-ray diffraction. This allows us to measure the thermal expansion at the atomic scale and to associate it with specific atomic pairs. Fe-Fe pairs are found to be responsible for the Invar effect at the atomic scale. Moreover, also full atomic shells, which contain all atomic species, show an abrupt increase in their thermal expansion. This proves that the Invar effect is not just a macroscopic effect but has clear origins at the atomic scale.

MM 30.7 Thu 12:00 H46

Coupling deformation mechanisms in metallic glass-high entropy alloy nanolaminates — ●QI XU¹, DANIEL ŞOPU¹, and JÜRGEN ECKERT^{1,2} — ¹Erich Schmid Institute of Materials Science, Leoben, Austria — ²Montanuniversität leoben, Leoben, Austria

The uniaxial tensile deformation behavior of metallic glass (MG) - high entropy alloy (HEA) nanolaminates is explored through molecular dynamics simulations. The combination of glassy and crystalline nanolayers results in misfit stresses at the interface that drive the partial crystallization of amorphous phase and the nucleation of short dislocations. Upon loading, the further stress-induced crystallization facilitates the nucleation and growth of dislocations along the interfacial regions and across the HEA plate, which advances the yielding of MG-HEA nanolaminate. The dislocations are absorbed into the amorphous plate via slip transfer across glass-crystalline interface that in turn triggers the activation of homogeneously distributed STZs. The co-deformation mechanism suppresses the formation of critical shear bands and increases the resistance to dislocation motion that, consequently, promotes enhanced ductility in MG-HEA nanolaminate. The strength combination of HEA and MGs and the complex deformation behavior may overcome the typical strength-ductility trade-off and make MG-HEA laminates promising candidates for a variety of structural and functional applications.

MM 30.8 Thu 12:15 H46

Tracer diffusion of Fe and Zr in CuZr nanoglasses — ●CHRISTIAN AARON RIGONI¹, HENDRIK VOIGT¹, EVGENIY BOLTYNJUK², BONNIE TYLER³, SERGIY DIVINSKI¹, HORST HAHN², and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — ³Physikalisches Institut, University of Münster, Germany

Metallic nanoglasses consist of nanometer-sized amorphous regions separated by amorphous interfaces. According to the current knowledge, the amorphous structure of these interfaces is different from that of the amorphous grains. This rather new class of material shows a different behaviour in comparison to conventional homogenous metallic glasses, e.g. a reduced density, a reduced number of nearest neighbor atoms, a different electronic structure, an increase in the ferromagnetic transition temperature and an increased thermal stability were reported. In the present work, tracer diffusion in CuZr nanoglasses and their homogenous amorphous counterparts is measured. For the investigation, a radiotracer technique via ion beam sputtering (⁸⁹Zr and ⁵⁵Fe radioisotopes) is applied as well as SIMS profiling using stable isotopes. The tracer diffusion measurements are demonstrated to represent a specific and sensitive probe of the structure modifications, and the results are compared to the observations made by TEM and APT.

MM 30.9 Thu 12:30 H46

Anomalous Liquids on a New Landscape: from Water to Phase-Change Materials — ●SHUAI WEI — Aarhus University, Aarhus, Denmark

A liquid that is cooled below its melting temperature, referred to as a supercooled liquid, can solidify into an amorphous rigid state (i.e., glass), if cooling is fast enough and crystallization is avoided. The phenomenology of supercooled liquids has been in general established. However, there are pronounced exceptions (e.g., water) which do not fall into the class of "normal" liquids but exhibit a transition behavior in their liquid states. The latest advances connect the unusual aspect of liquids to the properties of Phase-Change Materials (PCMs) that are the basis for non-volatile memory and neuromorphic technologies. Here we demonstrate that the "water-like" liquid anomalies exist in many alloys based on group-IV, V, VI elements including technologically important PCMs. Heat capacity, density, and thermal expansivity maxima were observed in the (supercooled) liquid states of those alloys. Structural changes were monitored using in-situ X-ray scattering and femtosecond X-ray diffractions. Dynamic properties were characterized by quasi-elastic neutrons scattering. Their anomalous behav-

iors can be rationalized in terms of liquid-liquid (metal-semiconductor, and fragile-strong) transitions. These transition behaviors have important implications for understanding the unusual phase switching behaviors in PCMs, in which amorphous phase can crystallize rapidly within tens of nanoseconds at an elevated temperature, while it retains excellent amorphous stability for 10 years at room temperature.

MM 30.10 Thu 12:45 H46

Thermophysical study of anomalies and transitions in liquid Bi-Ga and Ga-In systems — •YURI KIRSHON¹, SHIR BEN-SHALOM¹, MORAN EMUNA², YARON GREENBERG², EYAL YAHEL², and GUY MAKOV¹ — ¹Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — ²Physics Department, Nuclear Research Centre-Negev, Beer-Sheva 84190, Israel

Interest in the properties and applications of liquid metals has been reignited and leading to innovative new pathways. Work on low-

melting alloys provided new products such as Galinstan liquid metal thermometers, self-healing electronic devices and cooling systems for high-temperature reactors. However, due to the experimental challenges, study of thermophysical properties of liquid binary systems remains limited. In particular, Bi-Ga and Ga-In alloys have attracted scientific interest due to possible changes in their liquid structure, reported recently [Q.Yu (2017), Z.Wang (2017), Y.Kirshon (2019)]. In the present contribution, we report on thermophysical measurements conducted on Bi-Ga and Ga-In alloys. Custom table-top resistivity and differential thermal analysis (DTA) setups are presented, including a demonstration of their capability to capture subtle transitions in the melts. We observed evidence of liquid-liquid crossover in the liquid Ga-In, measured both systems at a temperature range in good agreement with previous density measurements. In the Bi-Ga system, we probed the liquid-liquid miscibility gap and were able to obtain the latent heat and resistivity change during the liquid de-mixing process. Both results were in good agreement with previous reports.

MM 31: Computational Materials Modelling: Physics of Ensembles 2

Time: Thursday 11:45–13:00

Location: H44

MM 31.1 Thu 11:45 H44

Making low-scaling GW accurate — •JAN WILHELM¹ and DOROTHEA GOLZE² — ¹Institute of Theoretical Physics, University of Regensburg — ²Faculty of Chemistry and Food Chemistry, TU Dresden

In standard GW implementations, the computational cost is growing as $O(N^4)$ in the system size N , which prohibits their application to many systems of interest. I present a GW algorithm in a Gaussian-type basis with a computational cost that scales with N^2 to N^3 . It will be shown that large minimax grids and resolution of the identity with the truncated Coulomb metric improve the accuracy of the low-scaling GW algorithm to < 0.01 eV for the GW100 test set. Large-scale applications of low-scaling GW will be discussed.

MM 31.2 Thu 12:00 H44

Atomic cluster expansion parametrization of carbon for a fast, accurate and transferable interatomic potential — •MINAAM QAMAR, MATOUS MROVEC, YURY LYSOGORSKIY, ANTON BOCHKAREV, and RALF DRAUTZ — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

We present a parametrization of the atomic cluster expansion (ACE) for carbon that can be employed in large-scale atomistic simulations of complex phenomena. The ACE model is parametrized over an exhaustive dataset of important carbon structures at extended volume and energy ranges, computed using highly accurate density functional theory (DFT). Dispersion corrections are explicitly added to properly account for long-ranged van der Waals interactions. A rigorous validation against DFT data reveals that ACE predicts accurately a broad range of properties of both crystalline and amorphous C phases while being significantly more computationally efficient than other popular machine learning models. We demonstrate the predictive power of ACE on two distinct applications: (1) brittle crack propagation in diamond at finite temperature, and (2) evolution of amorphous carbon structures at different densities and quench rates.

MM 31.3 Thu 12:15 H44

Design and analysis of scattering data driven molecular dynamics simulation on the example of water and selected crystals — •VERONIKA REICH¹, SEBASTIAN BUSCH¹, and MARTIN MÜLLER² — ¹German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Lichtenbergstr. 1, 85748 Garching bei München, Germany — ²Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Molecular dynamics simulations are an indispensable tool to preinvestigate neutron scattering experiments. For many systems reliable force fields have been established and yield to significant simulations. On the other hand a lot of systems still don't have a satisfactory agreement between experiment and simulation.

In this work we compare experimental data to different liquid water model simulations and give an outline to crystal simulations.

We simulate the samples using molecular dynamics simulations using the program LAMMPS. Subsequently we calculate the coherent and incoherent scattering signals using the program SASSENA. Ensuing we compare the outcomes to already existing experimental data and evaluate changes in the underlying force fields in terms of their impact on the behaviour of the simulation. Finally we compare the incoherent calculations to mathematical models, which in turn we later fit to the simulation.

The aim of our work is to create a simple to use workflow of molecular dynamics simulations for scattering experiments.

MM 31.4 Thu 12:30 H44

Approximating nuclear quantum effects in solids by temperature remapping — •RAYNOL DSOUZA¹, LIAM HUBER¹, BLAZEJ GRABOWSKI², and JÖRG NEUGEBAUER¹ — ¹Max Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — ²University of Stuttgart, 70569 Stuttgart, Germany

The quantum nature of solids, which is especially important at low temperatures, is often ignored in finite temperature atomistic simulations. Formulations to estimate quantum anharmonic effects precisely, such as the path integral method, are computationally demanding. Although various acceleration approaches allowing quantum effects to be fully accounted for in systems of hundreds of atoms have been proposed over the last two decades, they can fall short when it comes to modeling defects in solids, which can require significantly larger system sizes. We present a new approach for approximating nuclear quantum effects, exploiting a temperature map between the quantum system and its best classical surrogate. This map is constructed using the internal energies of classical and quantum harmonic oscillators within the Debye model. To a good approximation, our approach captures the impact of quantum effects on lattice constants, internal energies, and heat capacities with almost no additional cost compared to purely classical molecular dynamics simulations. Results for diamond cubic carbon and silicon are in good agreement with available literature values, which use full path integral Monte-Carlo simulations. We also show how this approach can be used to predict phase transition temperatures, e.g. the FCC to BCC transition for calcium.

MM 31.5 Thu 12:45 H44

Sharp phase-field modeling of isotropic solidification with a super efficient spatial resolution — •MICHAEL FLECK and FELIX SCHLEIFER — University of Bayreuth, 95447 Bayreuth, Germany

The phase-field method provides a powerful framework for microstructure evolution modeling in complex systems, as often required within the framework of integrated computational materials engineering. However, spurious grid friction, pinning and grid anisotropy seriously limit the resolution efficiency and accuracy of these models. The energetic resolution limit is determined by the maximum dimensionless driving force at which reasonable model operation is still ensured. This limit turns out to be on the order of 1 for conventional phase-field models. Grid friction and pinning can be eliminated by the restoration of Translational Invariance (TI) in the discretized phase-field equation. This is called the sharp phase-field method, which allows to choose sub-

stantially coarser numerical resolutions of the diffuse interface without the appearance pinning. We propose an accurate scheme to restore TI locally in the local interface normal direction. The new model overcomes grid friction and pinning in three dimensional simulations, and can accurately operate at dimensionless driving forces up to the order of 10^4 . At one-grid-point interface resolutions, exceptional degrees

of isotropy can be achieved, if further the inhomogeneous latent heat release at the advancing solid-liquid interface is mitigated. Imposing a newly proposed source term regularization the new model captures the formation of isotropic seaweed structures without spurious dendritic selection by grid anisotropy.

MM 32: Nanomaterials: Surface Effects

Time: Thursday 11:45–13:00

Location: H45

MM 32.1 Thu 11:45 H45

Effects of post anodization processes on the surface stability of anodic aluminum oxide — ●LYDIA DAUM, STEFAN OSTENDORP, and GERHARD WILDE — Westfälische-Wilhelms-Universität, Münster, Germany

The wide spectrum of different aluminum alloys enables the industry an economically advantageous material with the desired mechanical properties. In contrast to high-purity aluminum, the formation of a thin protective alumina layer is suppressed, which leads to a lower chemical corrosion resistance. Here anodization and the generation of anodic aluminum oxides (AAOs) are mandatory to obtain a necessary protective coating. The participating alloying elements are obstacles for mechanical stresses inside the AAOs which promotes the formation of nano- and microcracks at the surface. Thus, chemical attacks of the aluminum alloy are more favorable.

The use of post anodization processes will densify the pores and flatten the surface, which enhances the chemical resistance. A combination of nanoindentation studies and electron microscopy measurements are analyzing the surface stability of AAOs. By varying the methods in duration and medium, different wear, hardness and ductility characteristics are visible.

MM 32.2 Thu 12:00 H45

Surfaces of nanoporous gold: rough and faceted? — ●STEFAN A. BERGER¹, ULRIKE DETTE^{1,2}, LINGZHI LIU³, JÜRGEN MARKMANN^{1,2}, and JÖRG WEISSMÜLLER^{2,1} — ¹Helmholtz Zentrum Hereon — ²Technische Universität Hamburg — ³Shenyang National Laboratory for Materials Science

Nanoporous gold is an interesting model system for studying the impact of surfaces on the properties of nanomaterials. The surface morphology, faceted or rough, is of interest in that context. Scanning electron micrographs almost invariably show smoothly curved surfaces at the scale of the ligament size, suggesting roughness as opposed to faceting. Here, we show that proper imaging conditions to reveal facets, suggesting that the roughness may be an artifact of imaging. We find that the roughness is most pronounced after annealing in oxygen atmosphere. While low index facets are expected to prevail on gold, we regularly also observe high index facets.

MM 32.3 Thu 12:15 H45

Understanding of the underlying field evaporation mechanism of pure water tips in high electric fields — ●TIM MAXIMILIAN SCHWARZ¹, GUIDO SCHMITZ¹, NICO SEGRETO², JOHANNES KÄSTNER², and PATRICK STENDER¹ — ¹University of Stuttgart, Institute for Materials Science, Chair of Materials Physics, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²University of Stuttgart, Institute for Theoretical Chemistry, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Frozen liquids are challenging and rather new in the investigation by atom probe tomography. However, recent progress in instrumentation, especially the introduction of cryo transfer shuttles, and the development of the required preparation routes to shape nanometric needles of frozen liquids enable measurements of sufficient quality and size of data sets to discover the typical features of this material class. In this talk, we present the fragmentation behaviour of bulk frozen water as an important matrix for biomolecules or solvent of electrolytes. The obtained mass spectra are complex. However, this support of DFT calculations of the molecule stabilities, we identify a systematic series of protonated (H₂O)nH₃O⁺ events that represent a clear "fingerprint"

for the existence of water. Remarkably, tailing and the exact mass position of the two series differ, which provides evidence that the protonated fragments are permanently positively charged and therefore, slightly drawn out of the dielectric surface before the evaporation event.

MM 32.4 Thu 12:30 H45

Synthesis of superparamagnetic iron oxide nanoparticles by electron beam irradiation — ●JOHANNES DIETRICH^{1,2} and STEFAN MAYR^{1,2} — ¹Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM), Permoserstraße 15, 04318 Leipzig — ²Universität Leipzig, Fakultät für Physik und Geowissenschaften, Abteilung Oberflächenphysik, Linnéstraße 5, 04103 Leipzig

Nanoparticles based on iron oxides are a highly versatile material used in a broad range of applications, for instance embedding magnetic particles in polymer matrices to create ferrogels. A common procedure is to synthesize the particles in separate processes, add them to the gel and crosslink the polymer chains with nanoparticles by electron beam treatment. Combining synthesis and crosslinking would offer the possibility to create ferrogels by an one-step process.

In our work, we show a procedure to synthesize superparamagnetic nanoparticles with a narrow size distribution and an average size of approximately 5 nm directly by electron beam irradiation. The formation of small amounts of nanoparticles could already observed for doses of 50 kGy, but these particles showed a low crystallinity and a higher percentage of amorphous particles. For higher doses increasing crystallinity and yield could be observed, which is also reflected in the higher saturation magnetization for samples irradiated with higher doses. Additionally, particles irradiated with doses starting from 150 kGy show a tendency to form bigger cluster with sizes from 34 nm to 73 nm.

MM 32.5 Thu 12:45 H45

Probing the oxide formation on Pt, Pd and Pt/Pd catalysts during NO oxidation by Atom Probe Tomography (APT) — ●YOONHEE LEE¹, DANIEL DOBESCH², UTE TUTTLIES², PATRICK STENDER¹, ULRICH NIEKEN², and GUIDO SCHMITZ¹ — ¹Institute of Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²Institute of Chemical Process Engineering, University of Stuttgart, Böblinger Str. 78, 70199 Stuttgart, Germany *Yoonhee.lee@mp.imw.uni-stuttgart.de

Inverse hysteresis behavior of Pt, Pd and PtPd alloy catalysts during NO conversion can be attributed to the formation of metal oxides. Even though there were many efforts to study the oxidation of these noble metals experimentally, still the surface change of the pure catalyst has not been observed yet. In this work, NO conversion measurements were carried out with nanoparticles of Pt, Pd and Pt/Pd alloy, produced by spark discharge method, in an isothermal flatbed reactor. The catalyst was subjected to alternating heating and cooling ramps in conditions prone to surface oxide formation. Besides, the oxygen content formed on the surface of catalyst was determined during Temperature-Programmed Reduction (TPR) in H₂ atmosphere. The same conditions (gas concentration, heating and cooling rate) of the NO conversion experiments have been achieved in a reaction chamber directly connected to the Atom Probe Tomography (APT) under ultra-high vacuum conditions. The samples were exposed to the gas and measured in APT. The 3D chemical structure was reconstructed and the effective thickness of formed oxides was determined.

MM 33: Computational Materials Modelling: Process Schemes / Oxides

Time: Thursday 15:45–18:30

Location: H44

MM 33.1 Thu 15:45 H44

How to Speed up First-Principles Based Geometry Optimization with Small Numerical Basis Sets — ●ELISABETH KELLER, JOHANNES T. MARGRAF, and KARSTEN REUTER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

First-principles based geometry optimizations are often the most expensive part of high-throughput virtual screening studies for functional materials. This is particularly true for large systems, i.e. when studying complex surface reconstructions or nanoparticles. Here, the computational cost is strongly influenced by the size of the basis set. Large, converged basis sets result in precise equilibrium geometries, yet demand high computational cost and thus limit the simulation scale. Semiempirical methods using minimal basis sets offer a much lower computational cost, but may yield unacceptably large and uncontrolled errors. Furthermore, the availability of adequate parameterizations is rather sparse across the periodic table.

In this presentation, we will discuss the potential of using near-minimal basis sets for accelerating and enabling large-scale geometry optimizations at the DFT level. For this purpose, we studied how the size of the numeric atom-centered orbital (NAO) basis set in FHI-aims impacts the accuracy of bulk geometries. We recover equilibrium geometries at a nearly converged level with a highly compact basis by employing a simple short-ranged pair-potential correction. We show the scheme's ability to treat different systems across the periodic table ranging from small molecules and clusters to large-scale bulk and surface structures as well as complex molecule-surface interactions.

MM 33.2 Thu 16:00 H44

A machine-learned interatomic potential for crystalline and amorphous silica — ●LINUS ERHARD¹, JOCHEN ROHRER¹, KARSTEN ALBE¹, and VOLKER DERINGER² — ¹Institute of Materials Science, Technische Universität Darmstadt, Otto-Berndt-Strasse 3, 64287 Darmstadt, Germany — ²Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford OX1 3QR, United Kingdom

Fitting an interatomic potential for silicon oxide that can be used for both the amorphous and numerous crystalline phases has proven to be difficult. This is already shown by the large number of interatomic potentials published in the last decades. Here, we present a machine-learned interatomic potential for silica, which is highly transferable between different crystalline polymorphs and the amorphous phase. It predicts the thermodynamics of the system accurately and is able to generate low-defect amorphous models by melt and quench simulations. We also discuss the importance of choosing an appropriated exchange-correlation functional for density-functional data input, which is particularly important for silica. Since the generation of realistic amorphous structure models by melt-quench simulations is highly dependent on the quench rate, we show new ways via hybrid simulations that combine the speed of classical interatomic potentials with the accuracy of machine-learning potentials. We also investigate the extrapolation behavior of our machine-learning potential using high-pressure simulations. Finally, we show first steps towards an interatomic potential for mixed Si-SiO₂ systems.

MM 33.3 Thu 16:15 H44

An all-functionals automatic workflow for IR and Raman spectra — ●LORENZO BASTONERO¹ and LORENZO BASTONERO^{1,2} — ¹University of Bremen, Bremen, Germany — ²EPFL, Lausanne, Switzerland

IR and Raman spectroscopies are among the best methods for the characterisation of materials at small scales, thanks to their fast measurement and high sensibility to local composition and configuration. Theoretical calculations are fundamental for the interpretation of experimental results and for the assessment of thermal properties. DFT has been employed in the last decades as a reliable tool for the analysis of these spectra, although the calculation of vibrational properties has been limited to the use of few functionals. Here, we devise an automatic user-friendly workflow for IR and Raman calculations within the AiiDA infrastructure, which exploits the finite displacements and finite fields to allow application to any complex functional. The package provides at the same time easy access and full customisability, relevant both for less experienced users and more elaborate purposes such as

high-throughput searches.

MM 33.4 Thu 16:30 H44

A Workflow for Obtaining Robust Density Functional Tight Binding Parameters Across the Periodic Table — ●MENGHAN CUI, JOHANNES T. MARGRAF, and KARSTEN REUTER — Fritz-Haber-Institut der MPG, Berlin, Germany

The Density Functional Tight Binding (DFTB) approach allows electronic structure based simulations at length and time scales far beyond what is possible with first-principles methods. This is achieved by using minimal basis-sets and empirical approximations. Unfortunately, the sparse availability of parameters across the periodic table is a significant barrier to the use of DFTB in many cases.

In this contribution, we therefore propose a workflow which allows the robust and consistent parameterization of DFTB across the periodic table. Importantly, the approach requires no element-pairwise parameters and can thus easily be extended to new elements. Specifically, the parameters defining the band energy and repulsive potential are obtained via Bayesian Optimization on a set of elemental solids. In this way, robust baseline parameters can be obtained for arbitrary element combinations. The transferability of the parameters and applications in hybrid DFTB/Machine Learning models will be discussed.

MM 33.5 Thu 16:45 H44

ChemiTEM - optimized solutions and workflows for electron microscopy in materials science and chemistry — ●WALID HETABA^{1,2}, ROBERT IMLAU³, LISETH DUARTE-CORREA², MAXIMILIAN LAMOTH², STEPHAN KUJAWA³, and THOMAS LUNKENBEIN² — ¹Max-Planck-Institut für Chemische Energiekonversion, Mülheim/Ruhr, Deutschland — ²Fritz-Haber-Institut der MPG, Berlin, Deutschland — ³Thermo Fisher Scientific, Eindhoven, Niederlande

Transmission electron microscopy (TEM) is an important and versatile method for investigating materials on the nanoscale. Information about the elemental composition and electronic structure can be obtained while imaging the sample with atomic resolution. Such investigations are usually performed by TEM-experts. However, enabling non-expert TEM users to perform such measurements would tremendously improve the efficiency of TEM investigations in both, materials science and chemistry. We therefore developed ChemiTEM: a set of standardized workflows for data acquisition and analysis which are integrated in an app for tablets and smartphones to provide easy access for all TEM users, irrespective of their level of experience. We tested the ability of ChemiTEM in helping non-expert TEM users to collect high quality data by having non-expert and expert TEM users investigate the same sample. Using ChemiTEM, the data acquired by the non-expert users were of similar quality to that of the data recorded by the TEM-expert. Thus, we were able to show that using the ChemiTEM app, TEM can be made available to everyone working in materials science.

15 min. break

MM 33.6 Thu 17:15 H44

Determination of Formation Energies and Phase Diagrams of Transition Metal Oxides with DFT+U — ●DANIEL MUTTER¹, DANIEL URBAN¹, and CHRISTIAN ELSÄSSER^{1,2} — ¹Fraunhofer IWM, Freiburg, Germany — ²Freiburger Materialforschungsinstitut (FMF), Freiburg, Germany

Knowledge about formation energies of compounds is essential to derive phase diagrams of multicomponent phases with respect to elemental reservoirs. The determination of formation energies using (semi-)local exchange-correlation approximations of the density functional theory exhibits well-known systematic errors if applied to oxide compounds containing transition metal elements. We generalize and reevaluate a set of approaches proposed and widely applied in the literature to correct for errors arising from the over-binding of the O₂ molecule and from correlation effects of electrons in localized transition-metal orbitals. The DFT+U method is exemplarily applied to iron oxide compounds, and a procedure is presented to obtain the U values, which lead to formation energies and electronic band gaps comparable to the experimental values. Using such corrected formation energies, we derive phase diagrams for LaFeO₃, Li₅FeO₄, and NaFeO₂,

which are promising materials for energy conversion and storage devices. A scheme is presented to transform the variables of the phase diagrams from the chemical potentials of elemental phases to those of precursor compounds of a solid-state reaction, which represents the experimental synthesis process more appropriately. The workflow and methods can directly be applied to other transition metal oxides.

MM 33.7 Thu 17:30 H44

A comparative study of the bulk properties of iron oxides calculated using empirical potentials and ab-initio calculations

— ●AHMED ABDELKAWY, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Max-Planck-Str.1, 40470 Düsseldorf

Striving toward a green economy requires re-evaluating industrial processes and looking for new routes to, e.g., obtaining iron from iron ore. This necessitates understanding the steps involved in the reduction of iron oxides and leading to several phase transitions the final product of which is iron. The optimization of the involved processes will hugely benefit from an atomistic level understanding. Atomistic simulation techniques are versatile but are dependent on the quality of the used underlying empirical potentials. We therefore first evaluate the applicability of interatomic potentials for this study by comparing them to ab initio calculations. Specifically, we focus on a reactive forcefield (ReaxFF) parametrized for these materials, which accounts for the different oxidation states of each species (Fe and O) and enables their variation depending on the local environment and coordination, bond breaking, and making. We assess the reliability of the force field by assessing various bulk properties of the relevant iron as compared to density functional theory calculations. We find that a universal forcefield that is able to accurately describe the three main iron oxides (Magnetite, Hematite, and Wüstite) is difficult to obtain.

MM 33.8 Thu 17:45 H44

Uncertainty in Predicting Thermodynamic Properties of TiO₂ Polymorphs

— ●OLGA VINOGRADOVA, PIN-WEN GUAN, SIYING LI, and VENKATASUBRAMANIAN VISWANATHAN — Carnegie Mellon University, Pittsburgh, USA

Polymorphism of crystals directly leads to materials with vastly different chemical and physical properties. However the lowest energy polymorphs often differ by only small amounts of energy. This makes it challenging to predict relative properties using first-principles density functional theory (DFT), which is significant in designing a material for the desired application. In this work we apply computational uncertainty within DFT to quantify the accuracy of stability and phase transition predictions under finite temperature and pressure. We study six polymorphs of TiO₂ using a set of six exchange-correlation functionals to present a detailed sensitivity analysis using uncertainty capabilities within the Bayesian Error Estimation Functional. We show that a prediction confidence metric is particularly important for comparing the stability of numerically close predictions. We show how the choice of functional significantly affects predictions of phase transitions and identify which structures and properties that have inherently large uncertainties. From the trends observed in stability, finite-temperature, and phase transition pressure predictions we propose that uncertainty quantification provides a valuable insight in problems where drawn

conclusions are highly sensitive to the choice of the functional.

MM 33.9 Thu 18:00 H44

Self-consistent phonon calculations of lattice dynamical properties in cubic EuTiO₃ comparing with experimental thermal conductivity

— ●CHEN SHEN¹, WENJIE XIE¹, XINGXING XIAO¹, ANKE WEIDENKAFF¹, TERUMASA TADANO², and HONGBIN ZHANG¹ — ¹Institute of Materials Science, Technical University Darmstadt, Darmstadt 64287, Germany — ²Research Center for Magnetic and Spintronic Materials, National Institute for Materials and Science, Tsukuba, Japan

We investigate the role of the quartic anharmonicity in the lattice dynamics and thermal transport of the cubic EuTiO₃ by combining ab initio self-consistent phonon theory combined with compressive sensing techniques experimental thermal conductivity determination measurement. The antiferromagnetic G-type magnetic structure is used to mimic the para-magnetic EuTiO₃. We find that the strong quartic anharmonicity of oxygen atoms plays an essential role in the phonon quasiparticles free from imaginary frequencies in EuTiO₃, causing the hardening of vibrational frequencies soft modes. The hardened modes thereby affect calculated lattice thermal conductivity significantly, resulting in an improved agreement with experimental results, including the deviation from $\kappa_L \propto T^{-1}$ at high temperature. The calculated thermal conductivity of 8.2 W/mK at 300 K matched the experimental value of 6.1 W/mK. When considering the boundary scattering, the calculated thermal conductivity is reduced to 6.9 W/mK at 300 K, which agrees better with the experiment.

MM 33.10 Thu 18:15 H44

Simulated indentation on graphene oxide

— ●JAVIER ROJAS-NUNEZ¹, SAMUEL BALTAZAR¹, EDUARDO BRINGA², and ALEJANDRA GARCIA³ — ¹Physics Department and CEDENNA, Universidad de Santiago de Chile (USACH), Santiago, Chile — ²Laboratorio de síntesis y modificación de nanoestructuras y materiales bidimensionales, Centro de Investigación en Materiales Avanzados, Nuevo León, México — ³CONICET & Facultad de Ingeniería, Universidad de Mendoza, Mendoza, Argentina

The better understanding of nanomaterial properties will be a key factor to tailor and enhance properties of new materials. Graphene oxide in particular can be synthesized with different oxidation levels in order so gain similar properties to its deoxidized counterpart, graphene. Through the molecular dynamic simulations, the atomistic behavior of a tri-layer graphene membrane under mechanical indentation will be studied in this work.

This work will study a highly oxidized graphene oxide tri-layer that will be indented with a repulsive spherical indentator. The modeling of the membrane will generate single layer graphene oxide candidates to pick the lowest energy configuration and later stack this layer over itself. The final tri-layer was used for the indentation simulation, where the young modulus was reproduced with decent similarity to experimental results.

The atomistic analysis of the indentation process suggest an important role of epoxide groups in the mechanical deformation of the membrane.

MM 34: Data Driven Materials Science: Interatomic Potentials / Reduced Dimensions

Time: Thursday 15:45–18:30

Location: H45

MM 34.1 Thu 15:45 H45

Constructing Training Sets for Transferable Moment Tensor Potentials: Application to Defects in Bulk Mg

— ●MARVIN POUL, LIAM HUBER, ERIK BITZEK, and JOERG NEUGEBAUER — Max-Planck-Institut fuer Eisenforschung

Machine learned interatomic potentials promise to bring quantum mechanical accuracy to system sizes that are inaccessible with traditional QM approaches. Here, we present a set of unary Mg Moment Tensor Potentials[1] with different speeds and accuracies in the range of 100–5 meV/atom. We focus on understanding the role of the training data in the fitting process. We discuss several ways in which the structural complexity of the training structures and a physical understanding of them helps to design an efficient training set construction. The resulting potentials are verified on out-of-fold structures, like vacancies, sur-

faces, and high-symmetry grain boundaries. This work is implemented as a pyiron[2] workflow and we identify challenges and opportunities of a fully automated setup to fit machine-learned potentials.

[1]: <https://doi.org/10.1088/2632-2153/abc9fe>

[2]: <https://doi.org/10.1016/j.commatsci.2018.07.043>

MM 34.2 Thu 16:00 H45

Active learning and uncertainty quantification for atomic cluster expansion models

— ●YURY LYSOGORSKIY, ANTON BOCHKAREV, and RALF DRAUTZ — Atomistic Modelling and Simulation, ICAMS, Ruhr-University Bochum, D-44801 Bochum, Germany

Interatomic potentials (IP) are widely used in computational materials science, in particular for simulations that are too computationally expensive for density functional theory (DFT). Recently the atomic cluster expansion (ACE) was proposed as a new class of data-driven

IP with basis set completeness. Development of any IP requires numerous iterations and careful selection of training data. Thus automation of both construction of training dataset as well as IP validation would significantly speed up the development process. In this work we apply the Maxvol algorithm for training dataset selection and study the extrapolation grade metric (Podryabinkin and Shapeev, 2017) in the context of ACE and compare it to the query-by-committee approach for uncertainty estimation. These methods allow us to introduce extrapolation control in ACE models and to design different exploration automated protocols for accurate interatomic potentials development.

MM 34.3 Thu 16:15 H45

Take Two: Δ -Machine Learning for Molecular Co-Crystals — ●SIMON WENGERT^{1,2}, GÁBOR CSÁNYI³, KARSTEN REUTER¹, and JOHANNES T. MARGRAF¹ — ¹Fritz Haber Institut der MPG, Berlin, Germany — ²TU Munich, Germany — ³University of Cambridge, UK

Co-crystals are a highly interesting material class, as varying their components and stoichiometry in principle allows tuning supramolecular assemblies towards desired physical properties. The *in silico* prediction of co-crystal structures represents a daunting task, however, as they span a vast search space and usually feature large unit-cells. This requires theoretical models that are accurate and fast to evaluate, a combination that can in principle be accomplished by modern machine-learned (ML) potentials trained on first-principles data. Crucially, these ML potentials need to account for the description of long-range interactions, which are essential for the stability and structure of molecular crystals. In this contribution, we present a strategy for developing Δ -ML potentials for co-crystals, which use a physical baseline model to describe long-range interactions. The applicability of this approach is demonstrated for co-crystals of variable composition consisting of an active pharmaceutical ingredient and various co-formers. We find that the Δ -ML approach offers a strong and consistent improvement over the density-functional tight binding baseline. Importantly, this even holds true when extrapolating beyond the scope of the training set, for instance in molecular dynamics simulations at ambient conditions.

MM 34.4 Thu 16:30 H45

Magnetic Atomic Cluster Expansion and application to Iron — ●MATTEO RINALDI, MATOUS MROVEC, and RALF DRAUTZ — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

The atomic cluster expansion (ACE)^[1,2,3] has proven to be a valuable tool to parametrize complex energy landscapes of pure elements and alloys. However, its application to potential energy surfaces determined also by additional degrees of freedom, such as magnetic moments, has been still lacking. In particular, ferromagnetic materials cannot be tackled with the original ACE formalism, where the single-site energies depend parametrically only on interatomic distances and chemical species, since these descriptors cannot distinguish between atoms with different magnetic moments. The solution of this issue was given theoretically by Drautz^[4], where the ACE formalism was extended to take into account additional labels of the atomic sites of scalar, vectorial and tensorial nature by including them in the definition of the atomic neighbor density. We have employed this formalism to parametrize a magnetic ACE for the prototypical ferromagnetic element Fe using a dataset of both collinear and non-collinear magnetic structures calculated with spin density functional theory. We will show that the new ACE model is able to describe correctly not only various magnetic phases of Fe at 0 K but also their finite temperature properties in good agreement with the reference *ab-initio* and experimental values.

[1] R. Drautz, Phys. Rev. B 99, 014104. [2] Y. Lysogorskiy et al., npj Comput Mater 7, 97 (2021). [3] A. Bochkarev et al., Phys. Rev. Materials 6, 013804. [4] R. Drautz, Phys. Rev. B 102, 024104.

MM 34.5 Thu 16:45 H45

Kernel Charge Equilibration: Learning Charge Distributions in Materials and Molecules — ●MARTIN VONDRÁK, NIKHIL BAPAT, HENDRIK H. HEENEN, JOHANNES T. MARGRAF, and KARSTEN REUTER — Fritz-Haber-Institut, Berlin, Germany

Machine learning (ML) techniques have recently been shown to bridge the gap between accurate first-principles methods and computationally cheap empirical potentials. This is achieved by learning a systematic relationship between the structure of molecules and their physical properties. However, the modern ML models typically represent chemical systems in terms of local atomic environments. This inevitably leads to the neglect of long-range interactions (most prominently electrostatics) and non-local phenomena (e.g. charge transfer),

which can lead to significant errors in the description of polar molecules and materials (particularly in non-isotropic environments). To overcome these issues, we recently proposed a ML framework for predicting charge distributions in molecules termed Kernel Charge Equilibration (kQEq). Here, atomic charges are derived from a physical model using environment-dependent atomic electronegativities. These models can be trained to reproduce electrostatic properties (e.g. dipole moments) of reference systems, computed from first principles. The impact of different fitting targets on predicted charge distributions is compared. Furthermore, strategies for fitting to energies are discussed, including combination of Gaussian Approximation Potential (GAP) with kQEq.

15 min. break

MM 34.6 Thu 17:15 H45

Machine Learning of *ab-initio* grain boundary Segregation Energies — ●CHRISTOPH DÖSINGER¹, DANIEL SCHEIBER², OLEG PEIL², VSEVOLOD RAZUMOVSKIY², ALEXANDER REICHMANN¹, and LORENZ ROMANER¹ — ¹Montanuniversität Leoben, Department of Materials Science, Leoben, Austria — ²Materials Center Leoben Forschung GmbH, Leoben, Austria

Grain-boundary (GB) segregation is an important phenomenon in alloys, where the resulting GB excess can strongly influence their properties, for example induce intergranular fracture or lead to phase transformations. A fundamental quantity that uniquely describes the propensity of a solute towards GB segregation is the segregation energy. It determines the tendency of a solute atom to enrich or deplete at the GB. This quantity can be directly calculated from first principles. However, such calculations are computationally expensive and can become computationally unfeasible as the complexity of the GB crystal structure increases. The aim of this work is to reduce the computational cost of GB segregation energies by applying machine learning methods trained at series of representative DFT calculations and expanding them to more complex GB structures. The atomic structure, together with the segregation energies are used to train a model, which then is employed to predict the segregation energy for arbitrary segregation sites and GB types. In our work we apply this method to tungsten alloys. The results show, that this approach indeed gives reliable results for the segregation energies and can be used to get a complete description of segregation profiles.

MM 34.7 Thu 17:30 H45

Stability of binary precipitates in Cu-based alloys investigated through active learning and quantum computing — ●ANGEL DIAZ CARRAL¹, XIANG XU², AZADE YAZDAN YAR¹, SIEGFRIED SCHMAUDER², and MARIA FYTA¹ — ¹Institute for Computational Physics (ICP), Universität Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — ²Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Pfaffenwaldring 32 70569, Stuttgart, Germany

Understanding the structure of thermodynamically stable precipitates is of great interest in material science as they can affect the electrical conductivity and mechanical properties of the matrix to a great degree. In this work, we use a relaxation-on-the-fly active learning algorithm in order to scan all possible binary candidates, for different types and concentrations of alloy elements (mainly Cu, Si, and Ni). Quantum-mechanical calculations are performed on a small number of candidates to train and improve the machine-learned potential. The model is then used to predict the enthalpy of formation of all candidates. The stability of binary precipitates, based on predicting the convex hull, is further assessed by the phonon density of states analysis calculated by classic and quantum computing.

MM 34.8 Thu 17:45 H45

How to teach my deep generative model to create new RuO₂ surface structures? — ●PATRICIA KÖNIG, HANNA TÜRK, YONGHYUK LEE, CHIARA PANOSETTI, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz-Haber-Institut der MPG, Germany

Many widely used catalyst systems still hold complicated longstanding structural puzzles that hamper their full atomistic understanding and thus further knowledge based progress. Here, we address the well-known RuO₂ catalyst for the oxidative conversion of CO exhaust gases in combustion processes.

To explore the chemical space of RuO₂ surface structures, we trained a Generative Adversarial Network (GAN) that is capable of cheaply generating diverse structural guesses for novel surface structures. For

the training set, 28,903 RuO₂ surface terminations were created with a grand-canonical basin hopping method. The atomic positions of these structures were mapped to Gaussian densities on a three-dimensional grid to generate the GAN input. We demonstrate how two-dimensional images of cuts through RuO₂ structures with inferred lattice lengths and energy conditioning can be created as a first step to realistic three-dimensional surface structures.

MM 34.9 Thu 18:00 H45

Data-Driven Design of Two-Dimensional Non-van der Waals Materials — ●RICO FRIEDRICH^{1,2,3}, MAHDI GHORBANI-ASL¹, STEFANO CURTAROLO², and ARKADY V. KRASHENINNIKOV^{1,4} — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden — ²Duke University, Durham, USA — ³TU Dresden — ⁴Aalto University, Aalto, Finland

Two-dimensional (2D) materials are traditionally associated with the sheets forming bulk layered compounds bonded by weak van der Waals (vdW) forces. The weak inter-layer interaction leads to a natural structural separation of the 2D subunits in the crystals, giving rise to the possibility of mechanical and liquid-phase exfoliation as well as enabling the formulation of exfoliability descriptors.

The unexpected experimental realization of non-vdW 2D compounds, for which the previously developed descriptors are not applicable, opened up a new direction in the research on 2D systems [1]. Here, we present our recent data-driven search for representatives of this novel materials class [2]. By screening the AFLOW database according to structural prototypes, 28 potentially synthesizable candidates are outlined. The oxidation state of the surface cations is found to regulate the exfoliation energy with low oxidation numbers giving rise to weak bonding — thus providing an enabling descriptor to obtain novel 2D materials. The candidates showcase a diverse spectrum

of appealing electronic, optical and magnetic features.

- [1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).

MM 34.10 Thu 18:15 H45

Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning — ●ANDREAS LEITHERER, ANGELO ZILETTI, and LUCA M. GHIRINGHELLI — The NOMAD Laboratory at the Fritz Haber Institute and at the Humboldt University of Berlin, Germany

Atomic-resolution studies are routinely being performed in modern materials-science experiments. Artificial-intelligence tools are promising candidates to leverage this valuable – yet underutilized – data in unprecedented, automatic fashion to discover hidden patterns and eventually novel physics. Here, we introduce ARISE (Nat. Commun. 2021, <https://doi.org/10.1038/s41467-021-26511-5>), a crystal-structure-identification method based on Bayesian deep learning. As a major step forward, ARISE is robust to structural noise and can treat more than 100 crystal structures, a number that can be extended on demand. While being trained on ideal structures only, ARISE correctly characterizes strongly perturbed single- and polycrystalline systems, from both synthetic and experimental sources. The probabilistic nature of the Bayesian-deep-learning model yields principled uncertainty estimates, which are found to be correlated with crystalline order of metallic nanoparticles in electron-tomography experiments. Application of unsupervised learning to the internal neural-network representations reveals grain boundaries and (unapparent) structural regions sharing interpretable geometrical properties. This work enables the hitherto hindered analysis of noisy atomic structural data from computations or experiments.

MM 35: Nanomaterials: Structure & Properties

Time: Thursday 15:45–18:30

Location: H46

MM 35.1 Thu 15:45 H46

Structural and Electronic Reconstruction of Hexagonal Boron Nitride Interlayers Steps — ●SUBAKTI SUBAKTI^{1,2}, MOHAMMADREZA DAQIQSHIRAZI³, FELIX KERN^{1,2}, DANIEL WOLF¹, THOMAS BRUMME³, BERND BÜCHNER^{1,2}, and AXEL LUBK¹ — ¹Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — ²Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — ³Chair of Theoretical Chemistry, Technische Universität Dresden, Bergstrasse 66, 01069 Dresden, Germany

The electrostatic potential of condensed matter provides not only atomic structure, but also the electronic structure that underlies the chemical bonding formation of atoms within one molecule. Off-axis electron holography (EH) technique allows us to probe the volume-averaged electrostatic potential (in crystalline materials over the unit cell) of the specimen with respect to a vacuum reference region. Therefore, a conjunction EH medium and high resolution data analysis and electrostatic potential based ab-initio calculation will be powerful for simultaneous atomic scale reconstruction and imaging. Visible projected potential jump at the edges of two adjacent monolayers hexagonal boron nitride (h-BN) will be addressed here as our data analysis suggest that it could be signature for the increased charge delocalization due to the formation of an additional covalent bond of the 2p orbitals in the rolled-up edge.

MM 35.2 Thu 16:00 H46

Atom Probe Study of self-assembled Monolayers — ●HELENA SOLODENKO, PATRICK STENDER, and GUIDO SCHMITZ — University of Stuttgart, Institute for Materials Science, Heisenbergstr. 3, 70569 Stuttgart

Atom probe tomography is a well-established characterization technique for metals, semiconductors, oxides and minerals. However, measurement of organic matter and biological materials is still challenging. Field evaporation of organic species leads to detection of C_xH_y groups, instead of single atoms. The fragmentation of the molecules possibly depends on the applied electric field strength and the nature of chemical bonding. Self-assembled monolayers (SAMs) represent a suitable model system to study the fundamental questions about field evapora-

tion of such systems, since they represent a well-defined molecular film with a limited number of possible molecular fragments. Furthermore, a chemical bond is formed between substrate surface and the head-group the SAM. By variation of the field strength, we expect to learn more about the field evaporation process and thus about the binding energies of the SAMs. We present measurements of alkane-thiolates on Pt and silanes on ZnO by laser-assisted APT. The backbone evaporates in the form of small hydrocarbon fragments consisting of one to four C atoms, while S evaporates exclusively as single ions. With increasing laser power, a significant trend towards larger fragment sizes is observed. Furthermore, comparison with liquid alkanes and cross linked alkane networks is insightful which demonstrates a continuous transition from evaporation of complete molecules to single atoms.

MM 35.3 Thu 16:15 H46

Tuning the Electronic Properties of Mesocrystals — ●STEFAN MANUEL SCHUPP¹, CHRISTIAN JENEWEIN², BING NI², LUKAS SCHMIDT-MENDE¹, and HELMUT CÖLFEN² — ¹University of Konstanz, Department of Physics, Universitätsstraße 10, 78462 Konstanz, Germany — ²University of Konstanz, Department of Chemistry, Universitätsstraße 10, 78462 Konstanz, Germany

Colloidal crystals consisting of periodically aligned nanocrystalline building blocks, so-called mesocrystals, are promising candidates for nanostructured metamaterials. The high degree of order of the nanoparticles in the crystal results in a well-defined facet-to-facet distance which is determined by the used capping agents. In this work, we were able to grow micrometer-sized platinum nanocube-based mesocrystals with various capping agents and perform electrical measurements on individual crystals with a nanoprobe system. The extracted resistances increase with larger interparticle distances which can be attributed to the predominantly thermally activated tunneling mechanism in these superstructures. However, an additional annealing step leads to a decrease in resistance by seven orders of magnitude due to formed mineral bridges. After this treatment, the electronic properties are mainly determined by the nanomaterial itself. Finally, we were able to transfer these findings onto multi component superstructures consisting of platinum and iron oxide nanocubes. In these binary mesocrystals the ratio of the nanoparticle types can be varied to tune the electrical conductivity even further while simultaneously

allowing to combine properties of both nanomaterials.

MM 35.4 Thu 16:30 H46

Direct Visualization of Ordered Mesoporous Silica Using Atom Probe Tomography — ●KUAN MENG and GUIDO SCHMITZ — University of Stuttgart, Institute for Materials Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

Inspired by enzyme catalytic reaction, heterogeneous catalysis with mesoporous support materials is considered as the fundamental for modern chemical synthesis. However, the synergistic interplay between the catalysts and the pores is still unknown. To realize this, the structure of the mesoporous supports needs characterizing at first. Atom Probe Tomography, due to its subatomic resolution, strong chemical mapping power and direct visualization capability, is becoming a great candidate for mesoporous structure characterization. Yet to unfold its charm, pores must be filled.

In this work, Ordered Mesoporous Silica (OMS) filled with two different polymers, CDEAB and DCPD, was investigated. Firstly, both obtained mass spectra can be interpreted as a plausible combination of signature peaks between silica and polymers. Secondly, the porous network of OMS was visualized using neighboring analysis and the pore size turned out in the mesoporous range. Especially in the case of OMS filled with DCPD, the visualized network appeared to be regularly hexagonal, showing great resemblance with TEM images from similar pore orientations. Last, the obtained data were compared with the result of TAPsim simulations in order to understand the flaws in the visualization and to improve the understanding of the reconstructions.

MM 35.5 Thu 16:45 H46

plastic deformation of nanoporous gold modified with organic layers: a TEM study — ●XIN ZHANG and NADIA MAMEKA — Institute of Materials Mechanics, Helmholtz-Zentrum hereon, 21502 Geesthacht, Germany

As a result of their large specific surface area, strength of high-specific area materials must be sensitive to environment and surface chemistry. This notion is confirmed, e.g., by the enhanced flow stress found in single metal nanowires [1] and metallic networks like nanoporous metals when their surface is modified by adsorbed layers or surface coatings [2]. Yet, experimental studies of microstructural origins of the surface constraints impact on small-scale plasticity is still in its infancy. Here, we examine a defect structure of plastically deformed nanoporous gold (NPG) via ex-situ transmission electron microscopy. We exploit self-assembled monolayers (SAM) to modify a surface of NPG as inspired by a substantial flow stress increase due to SAM adsorption reported in [3]. In bare NPG deformed by rolling, we reveal higher density of twins consistent with [4]. In the deformed NPG with SAM, the formation of twins is strongly suppressed near the surface. Meanwhile, the existence of the organic layer apparently increases the density of twins in NPG. In the contribution, we discuss the TEM observations and link them to the findings from mechanical tests of the SAM-modified NPG. [1] Shin et al, Acta Mat. 166 (2019) 572e586. [2] Wu et al, Mater. Res. Lett. 6 (2018) 508. [3] Mameka et al, ACS Appl. Nano Mater. 1 (2018) 6613. [4] Liu, Weissmüller, Mater. Res. Lett. 9 (2021) 359.

15 min. break

MM 35.6 Thu 17:15 H46

Electrochemical actuation and tunable stiffness of hierarchical nanoporous gold via surface modification — ●OLGA MATTS and NADIA MAMEKA — Helmholtz-Zentrum Hereon, Geesthacht, Germany

Recently developed dealloying strategies towards nanoporous metals with structural hierarchy [1] open up new opportunities for functional behavior of this class of materials. The larger pores at the higher hierarchical level (characterized by diameters around 200 nm) of the hierarchical nanoporous metals (hc np) can promote fast mass exchange, while nanopores at the lower hierarchy level (below 30 nm) provide a large surface area. To explore the notion we employ electroactive self-assembled monolayers and conductive polymer polypyrrole for surface functionalization of hc np Au and np Au with unimodal pore size. Actuation and Young's modulus behavior of the hybrid materials were then analyzed in situ in a dynamical mechanical analyzer and dilatometer upon potential cycling in aqueous electrolytes. We revealed pronounced variations in the macroscopic length change as well as elastic

modulus in response to the voltage-induced redox reactions of the organic films at the np electrodes. In the contribution, we discuss the origin of the observations and compare the functional performance of both types of the hybrids based on np Au.

[1] Shi et al., Science 371, 1026*1033 (2021).

MM 35.7 Thu 17:30 H46

Laser-Ultrasonics Reveals the Complex Mechanics of Nanoporous Silicon — ●MARC THELEN¹, NICOLAS BOCHUD², MANUEL BRINKER¹, CLAIRE PRADA³, and PATRICK HUBER^{1,4,5} — ¹MXP, TUHH, Hamburg, Germany — ²MSME, CNRS UMR 8208, UPEC, Univ Gustave Eiffel, Creteil, France — ³Institut Langevin, ES-PCI Paris, Université PSL, CNRS, Paris, France — ⁴CXNS, DESY, Hamburg, Germany — ⁵CHyN, UHH, Hamburg, Germany

Nanoporosity in silicon leads to completely new functionalities of this mainstream semiconductor with numerous discoveries in fields ranging from nanofluidics and biosensorics to drug delivery, energy storage and photonics. Nevertheless, the mechanical properties, critical for a variety of applications, remain difficult to characterise comprehensively. The study presented here aims to address this problem by utilising laser-excited elastic guided waves, detected in dry and liquid-infused porous silicon. Among other things, the experiments reveal that the self-organised formation of 100 billions of parallel nanopores per square centimetre cross section results in an effective stiffness reduction of about 80 %, a nearly isotropic elasticity perpendicular to the pore axes and a higher stiffness along the pore axis, altogether leading to significant deviations from bulk silicon. This thorough assessment of the wafer-scale mechanics of nanoporous silicon and recent breakthroughs in laser ultrasonics therefore open up entirely new frontiers for in-situ, non-contact and non-destructive mechanical characterisation of complex porous material systems [1].

[1] Thelen, M., Bochud, N. et al., Nat Commun., 12, 3597 (2021)

MM 35.8 Thu 17:45 H46

Fabrication and compressive behavior of monolithic nanoporous niobium at macroscale — ●SEOYUN SOHN^{1,2}, SHAN SHI^{2,1}, JÜRGEN MARKMANN^{1,2}, and JÖRG WEISSMÜLLER^{2,1} — ¹Institute of Materials Mechanics, Helmholtz-Zentrum hereon, Geesthacht, Germany — ²Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Studying the mechanical performance of nanoporous (np) metals allows us to understand nanoscale solids as well as to design functional applications. However, the majority of studies have been confined to face-centered cubic noble metals such as gold and palladium due to high electronegativity which facilitates preparation by dealloying. Since the electrochemical or chemical dealloying involves a selective dissolution of less noble constituent(s) in an electrolyte solution, the remaining constituent should be nobler to form a bicontinuous porous structure. Niobium (Nb) on the other hand is less noble than gold, has higher stiffness and lower ductility, and its crystal lattice is body-centered cubic. In this work, np Nb was fabricated out of Ni75Nb25 by liquid metal dealloying; the ligament size could be controlled from 400 nm to more than 1 µm by adjusting dealloying time and temperature. Each sample body is a few mm in size and freestanding, which allows us to perform conventional macro-compression tests to measure the strength and stiffness of the nano-ligament scaffold. Our observations support that the material strength is enhanced with smaller ligaments. More interestingly, our np Nb shows extremely anomalous compliance.

MM 35.9 Thu 18:00 H46

Maximal Anderson Localization and Suppression of Surface Plasmons in Two-Dimensional Random Au Networks — ●JOHANNES SCHULTZ¹, KARL HIEKEL², PAVEL POTAPOV¹, PAVEL KHAVLYUK², ALEXANDER EYCHMÜLLER², and AXEL LUBK¹ — ¹Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — ²Chair of Physical Chemistry, TU Dresden, Zellescher Weg 19, 01069 Dresden, Germany

2D random metal networks possess unique electrical and optical properties, such as almost hundred percent optical transparencies and low sheet resistance, which are closely related to their disordered structure and may be exploited in various applications. Here we present a detailed experimental and theoretical investigation of their plasmonic properties, revealing Anderson (disorder-driven) localized surface plasmon (LSP) resonances of large quality factors and spatial localization close to the theoretical maximum. The LSPs typically consist of multiple field hotspots with a well-defined correlation distance. Moreover, they disappear above a geometry-dependent threshold at ca. 1.6 eV in

the investigated networks, explaining their large transparencies in the optical spectrum. Electron energy loss spectroscopy in combination with scanning transmission electron microscopy was applied for the experimental studies. Both, the high spatial (≈ 1 nm) and spectral (≈ 50 meV) resolution allows to study the variety of LSP modes in terms of excitation energy and spatial localization. The theoretical study is based on a coupled dipole model, which allows modeling of large plasmonic systems by exploiting Babinet's principle.

MM 35.10 Thu 18:15 H46

Laterally aligned nanowires: Targeted process design and alignment control — •JASMIN-CLARA BÜRGER, SEBASTIAN GUTSCH, and MARGIT ZACHARIAS — Laboratory for Nanotechnology, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 103, 79110 Freiburg, Germany

For sensors, tin oxide nanowires (NWs) have shown superior properties due to their unique geometry, which allows for high sensitivities. NWs

are often grown in freestanding mode for which metallization via standard lithography techniques is not applicable. In the production of single NW-based sensors, a multistep process has to be applied and an individual contacting of the NWs by, e.g., e-beam lithography becomes mandatory. Here, the use of planar NWs, i.e., laterally aligned NWs, is of advantage since the removal step from the growth substrate can be skipped and the NWs can be grown at defined positions. Due to their epitaxial contact with the monocrystalline growth substrate, the NWs are self-aligned towards the substrate lattice. However, the parameter space of these NWs is even smaller than for freestanding NWs. Based on finite element simulation and thermodynamic considerations, we developed a model for the growth of laterally aligned NWs.[1,2] The simulations and theory are supported by experimental results. Following, the preparation of longitudinal TEM lamella of individual NWs and AFM measurements allowed us for nanoscopic insight into the NW alignment on the growth substrate.[2]

[1] J.-C. Bürger et al., *Beilstein J. Nanotechnol.* (2020), 11, 843-853;
[2] J.-C. Bürger et al., *Cryst. Growth Des.* (2021), 21 (1), 191-199