

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 SCH A 118, SCH A 215, SCH A 216, and SCH A 251; Poster P2/OG1+2)

Invited Talks

MM 2.1	Mon	9:30–10:00	SCH A 251	Function follows form: on tailoring functional materials via microstructural design — ●ERICA LILLEODDEN
MM 7.1	Mon	15:00–15:30	SCH A 251	Molecular dynamics simulations of shock waves in alloys: Interplay of defects and phase transition — ●NINA MERKERT
MM 13.1	Tue	9:30–10:00	SCH A 251	Exploring the Slow Dynamics of Interfaces and Glasses via Markov State Models — SIAVASH SOLTANI, JOERG ROTTLER, ●CHAD SINCLAIR
MM 24.1	Wed	9:30–10:00	SCH A 251	Characterization of hydrogen effect on mechanical properties of metals at different length scales — ●AFROOZ BARNOUSH, PRINCE BARANWAL, HANAN FARHAT
MM 30.1	Wed	15:00–15:30	SCH A 251	Direct observations of grain boundary phase transformations in metallic alloys — ●CHRISTIAN LIEBSCHER

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	Diffusion of antibodies in solution: from individual proteins to phase separation domains — ●ANITA GIRELI
SYSD 1.2	Mon	10:00–10:30	HSZ 04	Intermediate Filament Mechanics Across Scales — ●ANNA V. SCHEPERS
SYSD 1.3	Mon	10:30–11:00	HSZ 04	Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition — ●JAN GERRIT HORSTMANN
SYSD 1.4	Mon	11:00–11:30	HSZ 04	Electro-active metasurfaces employing metal-to-insulator phase transitions — ●JULIAN KARST
SYSD 1.5	Mon	11:30–12:00	HSZ 04	The role of unconventional symmetries in the dynamics of many-body systems — ●PABLO SALA

Invited Talks of the joint Symposium Green Magnets for Efficient Energy Conversion (SYGM)

See SYGM for the full program of the symposium.

SYGM 1.1	Mon	15:00–15:30	HSZ 01	Data mining protocols for functional magnetic materials — ●OLLE ERIKSSON
SYGM 1.2	Mon	15:30–16:00	HSZ 01	High performance permanent magnets; elements criticality, new demands, and extrinsic magnetic properties — ●HOSSEIN SEPEHRI-AMIN, XIN TANG, TADAKATSU OHKUBO, KAZUHIRO HONO
SYGM 1.3	Mon	16:00–16:30	HSZ 01	Magnetic shape memory Heuslers: microstructure-related effects on the martensitic transformation — ●FRANCA ALBERTINI
SYGM 1.4	Mon	16:45–17:15	HSZ 01	Thin film combinatorial studies of hard magnetic materials — ●NORA DEMPSEY

SYGM 1.5	Mon	17:15–17:45	HSZ 01	Magnetocaloric materials for energy-efficient thermal control systems — •VICTORINO FRANCO, AUN N. KHAN, JORGE REVUELTA-LOSADA, ÁLVARO DÍAZ-GARCÍA, LUIS M. MORENO-RAMÍREZ, JIA YAN LAW
----------	-----	-------------	--------	---

Invited Talks of the joint Symposium Topological Superconductor-Magnet Heterostructures (SYTS)

See SYTS for the full program of the symposium.

SYTS 1.1	Thu	15:00–15:30	HSZ 01	Blending of superconductivity and magnetism via topological solitons — •CHRISTOS PANAGOPOULOS
SYTS 1.2	Thu	15:30–16:00	HSZ 01	Topological landscaping in magnet-superconductor heterostructures — •SEBASTIÁN A. DÍAZ
SYTS 1.3	Thu	16:00–16:30	HSZ 01	Experimental study of minigaps and end states in bottom-up designed multi-orbital Shiba chains — •JENS WIEBE
SYTS 1.4	Thu	16:45–17:15	HSZ 01	Quantum spins and hybridization in artificially-constructed chains of magnetic adatoms on superconducting 2H-NbSe₂ — •KATHARINA J. FRANKE
SYTS 1.5	Thu	17:15–17:45	HSZ 01	Braiding of Majorana zero modes — •STEPHAN RACHEL

Sessions

MM 1.1–1.1	Sun	16:00–18:00	HSZ 03	Hands-on Tutorial on Workflows for Materials Science Simulation (joint session MM/TUT)
MM 2.1–2.1	Mon	9:30–10:00	SCH A 251	Invited Talk: Lilleodden
MM 3.1–3.10	Mon	10:15–13:00	SCH A 251	Development of Computational Methods: Evaporation, Growth and Oxidation – Density Functional, Tight Binding
MM 4.1–4.7	Mon	10:15–13:00	SCH A 216	Topical Session: Fundamentals of Fracture – Micromechanical Fracture Experiments
MM 5.1–5.10	Mon	10:15–13:00	SCH A 215	Materials in Energy Conversion: Mechanical Properties and Solid State Batteries
MM 6.1–6.10	Mon	10:15–13:00	SCH A 118	Transport in Materials: Ion, Charge and Heat Transport
MM 7.1–7.1	Mon	15:00–15:30	SCH A 251	Invited Talk: Merkert
MM 8.1–8.7	Mon	15:45–17:45	SCH A 251	Development of Computational Methods: Diverse Topics and Machine Learning
MM 9.1–9.7	Mon	15:45–18:00	SCH A 216	Topical Session: Fundamentals of Fracture – Interface Fracture
MM 10.1–10.4	Mon	15:45–16:45	SCH A 215	Materials for Storage and Conversion of Energy: New Storage Materials
MM 11.1–11.5	Mon	17:00–18:15	SCH A 215	Functional Materials: Performance, Reliability and Degradation
MM 12.1–12.37	Mon	18:15–20:00	P2/OG1+2	Poster I
MM 13.1–13.1	Tue	9:30–10:00	SCH A 251	Invited Talk: Sinclair
MM 14.1–14.10	Tue	10:15–13:00	SCH A 251	Development of Computational Methods: Thermodynamics and Local Chemistry, Electronic Structure
MM 15.1–15.9	Tue	10:15–13:00	SCH A 216	Topical Session: Fundamentals of Fracture – Atomistic Studies of Fracture
MM 16.1–16.10	Tue	10:15–13:00	SCH A 215	Energy Conversion
MM 17.1–17.4	Tue	10:15–11:15	SCH A 118	Phase Transformations: Microstructural Transformations
MM 18.1–18.6	Tue	11:30–13:00	SCH A 118	Transport in Materials: Metals, Alloys and Oxides
MM 19.1–19.5	Tue	14:15–15:30	SCH A 251	Development of Computational Methods: Simulation Methods – Theory
MM 20.1–20.5	Tue	14:15–15:30	SCH A 216	Topical Session: Fundamentals of Fracture – Microstructure Impact on Fracture (Experiments)
MM 21.1–21.5	Tue	14:15–15:30	SCH A 215	Materials for Storage and Conversion of Energy: Energy Conversion
MM 22.1–22.6	Tue	14:15–15:45	SCH A 118	Mechanical Properties and Alloy Design: Porous and Nanostructured Materials
MM 23.1–23.35	Tue	18:15–20:00	P2/OG1+2	Poster II

MM 24.1–24.1	Wed	9:30–10:00	SCH A 251	Invited Talk: Barnoush
MM 25.1–25.5	Wed	10:15–11:30	SCH A 251	Development of Computational Methods: Crystal Structure and Properties
MM 26.1–26.10	Wed	10:15–13:00	SCH A 216	Interface Controlled Properties and Nanomaterials: Grain Boundaries and Stability, Spectroscopy and Interatomic Potentials
MM 27.1–27.10	Wed	10:15–13:00	SCH A 215	Hydrogen in Materials
MM 28.1–28.9	Wed	10:15–12:45	SCH A 118	Liquid and Amorphous Metals
MM 29.1–29.5	Wed	11:45–13:00	SCH A 251	Data Driven Materials Science: Big Data and Work Flows – Electronic Structure
MM 30.1–30.1	Wed	15:00–15:30	SCH A 251	Invited Talk: Liebscher
MM 31.1–31.10	Wed	15:45–18:30	SCH A 251	Data Driven Materials Science: Big Data and Work Flows – Machine Learning
MM 32.1–32.8	Wed	15:45–18:30	SCH A 216	Topical Session: Defect Phases I
MM 33.1–33.8	Wed	15:45–18:00	SCH A 215	Topical Session: Fundamentals of Fracture – Amorphous Metals
MM 34	Wed	18:45–19:45	SCH A 251	Members' Assembly
MM 35.1–35.1	Thu	9:30–10:00	SCH A 251	Invited Talk: Champion
MM 36.1–36.11	Thu	10:15–13:15	SCH A 251	Data Driven Materials Science: Big Data and Work Flows – Microstructure-Property-Relationships (joint session MM/CPP)
MM 37.1–37.8	Thu	10:15–13:00	SCH A 216	Topical Session: Defect Phases II
MM 38.1–38.3	Thu	10:15–11:15	SCH A 215	Topical Session: Fundamentals of Fracture – Fracture Experiments
MM 39.1–39.6	Thu	11:45–13:15	SCH A 215	Phase Transformations: Simulation and Machine Learning
MM 40.1–40.10	Thu	15:45–18:30	SCH A 251	Mechanical Properties and Alloy Design
MM 41.1–41.7	Thu	15:45–18:00	SCH A 216	Topical Session: Defect Phases III
MM 42.1–42.10	Thu	15:45–18:30	SCH A 215	Interface Controlled Properties and Nanomaterials: Nanoporous Materials and Nanolaminates

Members' Assembly of the Metal and Material Physics Division

Wednesday 18:45–19:45 SCH A 251

MM 1: Hands-on Tutorial on Workflows for Materials Science Simulation (joint session MM/TUT)

Time: Sunday 16:00–18:00

Location: HSZ 03

Tutorial MM 1.1 Sun 16:00 HSZ 03
Hands-on tutorial on workflows for materials science simulations — ●JÖRG NEUGEBAUER¹, TILMANN HICKEL¹, and RALF DRAUTZ² — ¹Max-Planck-Institut für Eisenforschung, Düsseldorf — ²ICAMS, Ruhr-Universität Bochum

Advanced computational simulations in materials science have reached a maturity that allows one to accurately describe and predict materials properties and processes. The underlying simulation tasks often involve several different models and software that requires expert knowledge to set up a project and to vary input parameters. The accompanying increasing complexity of simulation protocols means that the workflow along the simulation chain becomes an integral part of

research. Effective workflow management therefore is important for efficient research and transparent and reproducible results.

In this hands-on tutorial we will provide an interactive hands-on introduction into managing workflows with pyiron (www.pyiron.org). Pyiron is an integrated development environment for materials science built on python and Jupyter notebooks that may be used for a wide variety of simulation tasks, from rapid prototyping to high performance computing. The tutorial will first give a general introduction to using pyiron, with a focus on atomistic simulation tasks. In the second part of the tutorial, the training and validation of machine learning potentials from reference density functional calculations will provide a real-life application example.

MM 2: Invited Talk: Lilleodden

Time: Monday 9:30–10:00

Location: SCH A 251

Invited Talk MM 2.1 Mon 9:30 SCH A 251
Function follows form: on tailoring functional materials via microstructural design — ●ERICA LILLEODDEN — Fraunhofer-IMWS

While the Bauhaus adage says that form follows function, materials scientists understand that function follows form; we aim to exploit structuring of materials to achieve targeted function; the inherent interplay between processing, structure and properties is indeed the cornerstone

of materials science. In this talk, I will present two examples in which various structural elements can be used to tune the functional response of materials in ways that may be unexpected: exploiting structural geometry to tailor strength to stiffness ratios; and how alloying and thermal treatments can lead to a simultaneous increase in both strength and hardening. These examples will be placed in the context of how we view classical laws governing structure-property relations, with an outlook on new approaches to materials design going forward.

MM 3: Development of Computational Methods: Evaporation, Growth and Oxidation – Density Functional, Tight Binding

Time: Monday 10:15–13:00

Location: SCH A 251

MM 3.1 Mon 10:15 SCH A 251
Towards machine learning potentials for field evaporation — ●SHYAM KATNAGALLU, JOERG NEUGEBAUER, and CHRISTOPH FREYSOLDT — Department of computational materials design, Max Planck Institut für Eisenforschung GmbH, Düsseldorf, Germany.

Field evaporation, an electrostatic field-induced ionization and subsequent evaporation of surface atoms, is the underlying principle of atom probe tomography. Ab initio simulations including 1-10 V/Å fields on metallic slabs have recently shed light [1] on the intricacies of the field evaporation process. These simulations underscore the importance of knowing the path of the evaporating atom prior to complete ionization to improve the spatial resolution of the technique. However, to properly sample the extremely shallow potential energy surface due to the electrostatic field extensive simulations with computationally expensive ab initio accuracy are needed. We, therefore, combine machine learning interatomic potentials with a charge equilibration scheme. To demonstrate the performance and accuracy of our scheme, we validate the Rappe et al charge equilibration model [2] using Hirshfeld decomposed DFT reference charges acquired from (13,5,7) Pt slab under electric fields ranging from (1-4.5 V/Å) and develop potentials for field evaporation in Al. [1]*M. Ashton, A. Mishra, J. Neugebauer, and C. Freysoldt, Ab Initio Description of Bond Breaking in Large Electric Fields, Phys. Rev. Lett. 124, (2020). [2]*A. K. Rappe and W. A. G. III, Charge Equilibration for Molecular Dynamics Simulations, J. Phys. Chem 95, 3358 (1991).

MM 3.2 Mon 10:30 SCH A 251
High temperature chlorine corrosion in waste-to-energy-plants: sulphation of chloride particles as source of released chlorine — ●SEBASTIAN PENTZ, MATTHIAS KROH, and FERDINAND HAIDER — University of Augsburg, Chair for Experimental Physics I, Universitätsstr. 1, 86159 Augsburg

Chlorine induced high temperature corrosion leads to massive problems especially in waste-to-energy-plants. 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. For chloride particle sampling from a plant a tempered probe was developed, allowing time series of deposit built-up at defined temperatures. From this online particle sampling during plant operation we collect information about sticking probability, size distribution of deposited particles and the chemical composition of the deposit built up. Especially the relation between detected chlorine to sulphur is of high interest, leading to the degree of conversion of deposited chlorides, which equals the amount of released chlorine. In further laboratory experiments the sulphation process of synthetic chloride particles can be systematically studied. From this we get the sulphation kinetics under various conditions like temperature, particle size or gas composition, which lead to an estimation of the time required for full chloride conversion. By combining the results gained from laboratory experiments, online particle sampling and offline deposit analysis, we try to model the ongoing sulphation process.

MM 3.3 Mon 10:45 SCH A 251
How to teach my deep generative model to create new RuO₂ surface structures? — ●PATRICIA KÖNIG, HANNA TÜRK, YONGHYUK LEE, CHIARA PANOSSETTI, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz-Haber Institute, Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany

Data-driven approaches to inversely design novel materials with desired properties constitute an emerging pillar in the exploration of energy conversion materials. In recent works, artificial neural networks were successfully used to create crystalline porous materials. Here, we present a related approach to tackle the problem of structure generation for nano-porous to partially amorphous surfaces. As a model system, we use the well-studied RuO₂ catalyst for oxidative conversion of CO to CO₂. 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 termina-

tions were created with a grand-canonical basin hopping method using ML potential energetics. The atomic positions of these structures were mapped to Gaussian densities on a three-dimensional grid to generate the GAN input. We demonstrate how realistic three-dimensional surface models with inferred lattice lengths and energy conditioning can be created and how these generated densities can be mapped back to atomistic structures as a basis for property calculations.

MM 3.4 Mon 11:00 SCH A 251

Liquid-Diffusion-Limited Growth of Vanadium Dioxide Single-Crystals — ●NICO SPRINKART, DANIEL KAZENWADEL, ROMAN HARTMANN, and PETER BAUM — Department of Physics, University of Konstanz

Vanadium dioxide (VO_2) is a strongly correlated material with an ultrafast first-order phase transition between rutile/insulator and monoclinic/metallic close to room temperature. The unusual and complex properties of this transition make VO_2 one of the most heavily investigated materials in modern condensed matter physics. Consequently, high-quality single-crystals are in large demand.

Here we present a method for the growth of mm-sized stoichiometric VO_2 crystals by thermal decomposition of liquid V_2O_5 . Time-resolved measurements of the oxygen release reveal that the crystal growth rate is limited by liquid-phase diffusion; the properties of the gaseous environment, which were previously assumed to be decisive, are almost insignificant.

Our results signify the role of gas-liquid diffusion in crystal growth and will simplify future research on VO_2 and its subsequent application in ultrafast electronics and thermal energy management.

MM 3.5 Mon 11:15 SCH A 251

Dynamic restructuring of oxidation states in magnetite — ●EMRE GÜRSOY¹, GREGOR B. VONBUN-FELDBAUER², and ROBERT H. MEISSNER^{1,3} — ¹Institute of Polymer and Composites, Hamburg University of Technology, Hamburg, Germany — ²Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ³Institute of Surface Science, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Magnetite is a mineral that undergoes a metal-insulator transition called the Verwey transition at 125 K (T_V). Its conducting behaviour above T_V is linked to electron hops between Fe^{2+} and Fe^{3+} on octahedral sites and complex oxidation state patterns emerge as a direct consequence. Oxidation states are frequently assessed using quantum mechanical methods, but these computationally expensive methods are not scalable to relevant systems with several thousand atoms. Therefore, a computationally inexpensive method that provides a detailed atomistic description of magnetite would be beneficial. We present a hybrid Monte Carlo/Molecular Dynamics (MC/MD) approach for atomistic modeling of magnetite, magnetite surfaces, and nanoparticles that can capture many aspects of this oxidation state patterning. It is based on swapping the oxidation states of Fe ions using MC either in simulated annealing, or in a hybrid combination with MD. We confirmed the accuracy of our model by comparison with oxidation states determined from density functional theory. This simple yet efficient approach paves the way to elucidate aspects of oxidation state ordering and electron hopping in inverse spinel structures in general.

15 min. break

MM 3.6 Mon 11:45 SCH A 251

Role of an adsorbed gas layer in field ion microscopy contrast — ●SHALINI BHATT, FELIPE F. MORGADO, SHYAM KATNAGALLU, CHRISTOPH FREYSOLDT, and JÖRG NEUGEBAUER — Max Planck Institut für Eisenforschung GmbH Düsseldorf Germany

The imaging contrast in field ion microscopy (FIM) is associated with the ionization probability of gas atoms near a surface under 10-100 V/nm electric fields. To better understand contrast variations among atoms observed in FIM, we employ density functional theory (DFT) in combination with the Tersoff-Hamann approximation that links electron tunneling from the gas atom to the surface with the surface's local density of states at the position of the gas atom 3-6 Å away from the surface. Based on our new EXTRA approach (extrapolated tail via reverse algorithm) that eliminates numerical noise in the tails of the wavefunctions, we demonstrate a chemical brightness contrast for Ta in Ni (012) surface. However, we find that the simulated imaging contrast for Ni alone is much lower than in experiment. We therefore explore the role of an adsorbed gas layer as an essential ingredient to

explain FIM's unexpectedly large spatial resolution.

MM 3.7 Mon 12:00 SCH A 251

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 3.8 Mon 12:15 SCH A 251

Coupling Many Body Perturbation Theory (MBPT) with Polarizable Continuum Models (PCM) — ●PINO D'AMICO¹, DARIO A. LEON VALIDO², MARGHERITA MARSILI³, DANIELE VARSANO¹, STEFANO CORNI⁴, and ANDREA FERRETTI¹ — ¹S3 Center, Istituto Nanoscienze CNR, Modena, Italy — ²Dpt. REALTEK, Norw. Univ of Life Sci., Ås, Norway — ³Dpt. di Fisica e Astronomia, Univ. di Bologna, Italy — ⁴Dpt. di Scienze Chimiche, Univ. di Padova, Italy

The theoretical description of quantum systems embedded in external environments represents a challenge for the application of MBPT approaches to the study of the electronic excitations. Different level of accuracy can be used to treat the actual system, for which a quantum mechanical description is employed, and its surrounding environment, that can be approximated through a simplified quantum model, a molecular mechanical approach, or a continuum model. We will present a theoretical framework in which a MBPT treatment of the quantum system (eg at the level of GW and BSE) is coupled to a PCM description of its surrounding environment. The formalism has been implemented within the YAMBO code[1], based on plane-waves and pseudopotentials, by exploiting the ENVIRON package[2] coupled to the Quantum ESPRESSO suite[3]. Preliminary results of the newly developed methodology will be presented, focusing on selected molecules and two-dimensional materials in water. [1] D. Sangalli et al., J.of Phys.:Cond.Mat. 31, 325902 (19).[2] O. Andreussi et al., J.Chem.Phys. 136, 064102 (12).[3] P. Giannozzi et al., J.Phys.:Cond.Mat. 29, 465901 (17).

MM 3.9 Mon 12:30 SCH A 251

A DFTB-based approach to calculating electron-phonon couplings — ●ALEXANDER CROY¹, ELIF UNSAL², GIANAURELIO CUNIBERTI², and ALESSANDRO PECCHIA³ — ¹Institute of Physical Chemistry, FSU Jena, Germany — ²Institute of Materials Science, TU Dresden, Germany — ³Institute of Nanostructured Materials, CNR, Italy

The calculation of electron-phonon couplings from first principles is computationally very challenging and remains mostly out of reach for systems with a large number of atoms. Resorting to semi-empirical methods, like density-functional based tight-binding (DFTB), has been shown to be a viable approach for obtaining quantitative results at moderate computational costs. In this contribution, we present a method for calculating the electron-phonon coupling matrix within the DFTB approach and demonstrate its implementation which is based on dftb+ and phonopy. It further allows the calculation of relaxation times and interfaces with BoltzTrap2 to compute transport properties. Exemplarily, we show results for γ -graphyne which was recently synthesized. Consistent with earlier predictions we obtain mobilities on the order of $10^4 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ at room temperature.

MM 3.10 Mon 12:45 SCH A 251

Toward Coarse-Grained Elasticity of Single-Layer Covalent Organic Frameworks — ●DAVID BODESHEIM¹, ANTONIOS RAPTAKIS¹, AREZOO DIANAT¹, ALEXANDER CROY², and GIANAURELIO CUNIBERTI¹ — ¹TU Dresden, Dresden, Germany — ²FSU Jena, Jena, Germany

Covalent Organic Frameworks (COFs) are crystalline porous materials that are based on organic monomeric units, so called building blocks. As a multitude of different building blocks can be combined in reticular chemistry, manifold different porous structures with tailored properties have been synthesized in recent years. Through current experimental progress, monolayer COF materials have been synthesized, providing a new class of 2D materials.[1,2] However, these materials have defects and grain boundaries which make it challenging to describe properties of realistic materials computationally. To approach this issue, we show in this work how to use a surrogate model to calculate elastic

properties of 2D COFs based on density functional based tight binding (DFTB) calculations.[3] This allows us to model defective systems at low computational cost and paves the way for multiscale modeling. Furthermore, this approach enables us to predict elastic properties from the properties of the monomeric building blocks.

[1] A. Ortega-Guerrero, et al. ACS Appl. Mater. Interfaces, 13, 22, 26411-26420 (2021).

[3] Z. Wang, et al., Nat. Synth., 1, 69-76 (2022).

[3] A. Croy, et al. J. Phys. Chem. C, 126, 44, 18943-18951 (2022).

MM 4: Topical Session: Fundamentals of Fracture – Micromechanical Fracture Experiments

Time: Monday 10:15–13:00

Location: SCH A 216

Topical Talk

MM 4.1 Mon 10:15 SCH A 216

Crack and dislocations interactions: coupling DDD and XFEM — ELENA JOVER-CARRASCO¹, ERIK BITZEK², and ●MARC FIVEL¹ — ¹CNRS/SIMaP, Univ. Grenoble Alpes, Grenoble, France — ²MPIE, Computational Materials Design, Dusseldorf, Germany

The objective of this study is to build a numerical tool which could handle both cracks and dislocations in a dynamic manner. To do so, a 3D Discrete Dislocation Dynamics (DDD) code has been combined to the Extended Finite Element Method (X-FEM) via a strong coupling with the Finite Element software CAST3M. In the original FEM code, the crack advance is computed from the G- θ method which gives access to the stress intensity factors K. In this formalism, θ is the kinematically admissible virtual displacement of the crack and G is the energy release rate at the crack tip. When dislocations are present in the simulated box, they modify the evaluations of the energy and consequently the values of the derived stress intensity factors. These modifications are computed locally all along the crack front which is defined using level set functions. The crack front may locally change its direction of motion depending on the relative values of the stress intensity factors, especially KII. This will then lead to blunting effect of the crack tip.

In this presentation, full details of the coupling will be given. Test cases will then be presented where the behavior of a single dislocation in vicinity of a crack will be compared to atomistic simulations. Finally, large scale simulations of a mode I opening crack will be performed.

Topical Talk

MM 4.2 Mon 10:45 SCH A 216

multiscale studies on the fracture behaviors of body centered cubic metal — ●YINAN CUI, ZHIJIE LI, and ZHANGTAO LI — Applied Mechanics Lab., School of Aerospace Engineering, Tsinghua University, Beijing 100084, PR China

How the plasticity features influence the fracture behaviors of material is a critical question but remains far from well understood. To disclose this mystery, a multiscale plasticity-fracture coupled model is developed, which considers the atomistic-scale dislocation motion mechanism, the mesoscopic scales of discrete crack-dislocation interactions, and the continuum scale of crystalline plastic-fracture response. Body center cubic (bcc) material is chosen as an example to demonstrate the effectiveness of the developed model due to their wide applications and their special plasticity features, such as strong temperature dependence and non-Schmid effect. Several new insights about the fracture behavior of bcc material are gained.

MM 4.3 Mon 11:15 SCH A 216

Micro-cantilever experiments to study the influence of pre-deformation and He irradiation on the fracture toughness of W single crystals — STEFAN GABEL¹, MANUEL KÖBRICH¹, JAN VOLLHÜTER¹, BENEDIKT EGGLE-SIEVERS¹, BENOIT MERLE², ERIK BITZEK³, and ●MATHIAS GÖKEN¹ — ¹Friedrich-Alexander-University Erlangen-Nürnberg (FAU) — ²University Kassel — ³Max-Planck-Institut für Eisenforschung, Düsseldorf

Micro-cantilever fracture testing has been proven to be a very reliable method to determine the fracture toughness at the very small scale. In the work by Ast et al.[1] the influence of the specimen size on the fracture behavior of single and polycrystalline tungsten has been investigated in detail from which it can be concluded that the fracture toughness as analysed with the J-integral approach slightly increases with the specimen size. Here we focus on the brittle-to-ductile tran-

sition and the influence of pre-deformation and He irradiation on w single crystals. The fracture toughness is analysed in a temperature regime from 233 K up to 353 K with a FemtoTools in-situ nanoindentation system. Pre-deformation by compression in the <110>direction led to a population of specific glide systems. The results show depending on the sample orientation an increase of the hardness and a slightly higher fracture toughness at low temperatures. Irradiation by He+ ions clearly lead to a decrease of the fracture toughness although the hardness increases. The experimental results will be discussed in comparison with modelling results. [1] *J. Ast, M. Göken, K. Durst, Acta Materialia 138 (2017) 198-211

15 min. break

Topical Talk

MM 4.4 Mon 11:45 SCH A 216

Capturing Micromechanical Crack Tip Stress States and Toughening Plasticity in 2D and 3D — ●THOMAS E. J. EDWARDS¹, JOHANNES AST^{1,2}, SZILVIA KALÁCSKA^{1,3}, XAVIER MAEDER¹, JON WRIGHT⁴, and JOHANN MICHLER¹ — ¹Empa, Feuerwerkerstrasse 39, 3602 Thun, Switzerland — ²CEA, 17 rue des Martyrs, 38054 Grenoble, France — ³Mines Saint-Etienne, Univ Lyon, CNRS, UMR 5307 LGF, France — ⁴ESRF, 38000, Grenoble, France

Crack tip toughening mechanisms in metals require plasticity, i.e. slip; the present study sheds predictive light on what local stress states lead to an increased dissipation of mechanical energy through plasticity. It also confirms the notion that the plastic performance of a material cannot be solely interpreted from elastic strain measurements, even if undertaken in-situ, or from post-mortem TEM imaging of dislocation structures. Pre-notched single crystal W microcantilevers were deformed in situ, whilst elastic and total strains at the notch tip were captured correlatively by DIC and HR-EBSD with sub-100 nm resolution. From the basic elastic and total strains and rotations hence measured, as well as post-mortem TEM, the following could be extracted: maps of shear stresses resolved onto individual slip systems, pure plastic strain resolved onto slip axes and GND density - all throughout loading, as well as the total dislocation density of the near-surface layer post-mortem. Further, we demonstrate a novel method to extract the full stress tensor, point-wise in 3D, again with ~100 nm resolution, on micromechanical testpieces under load: nano-beam 3D-XRD computed tomography at ESRF ID11.

MM 4.5 Mon 12:15 SCH A 216

Size effect in fracture mechanics: a detailed investigation regarding crack initiation and growth on the micro- and mesoscale — ●JUTTA LUKSCH¹, ALOSHIOUS LAMBAL², GAURAV MOHANTY², FLORIAN SCHAEFER¹, and CHRISTIAN MOTZ¹ — ¹Materials Science and Methods, Saarland University, 66123 Saarbruecken, Germany — ²Materials Science and Environmental Engineering, Tampere University, 33014 Tampere, Finland

Fracture mechanics are strictly regulated by standards. This includes limitations of specimen size as a function of the plastic zone size that mainly depends on the material itself. Hence, established test procedures are not easily downscalable to nanomechanic testing. With progress in specimen preparation by FIB and test design e.g. in-situ testing in SEM, there are now ways to investigate a size effect systematically according crack initiation and growth. In the present study nanocrystalline nickel with a grain size of 40-50 nm is used as material to ensure a polycrystalline, quasi-homogeneous microstructure even for small samples. Micro bending beams of different dimensions are made using a FIB in order to study the fatigue size effect. Special

attention was laid to introduce a fatigue pre-crack into the sample by cyclic loading with $R < 0$ in a SEM with a nanoindenter. A study of crack initiation stress and number of needed cycles was made. The focus was given on microstructural changes. This pre-crack is then subjected to fatigue ($R > 0$) and crack growth is quantified by the compliance method. In addition, the stress intensity factor is evaluated and related to the crack growth.

MM 4.6 Mon 12:30 SCH A 216

Quantitative measurement of fracture toughness from the bridge notch failure in microcantilever — ●YINXIA ZHANG¹, MATTHIAS BARTOSIK², STEFFEN BRINCKMANN³, SUBIN LEE¹, and CHRISTOPH KIRCHLECHNER¹ — ¹Institute for Applied Materials, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, 76344, Germany — ²Department of Materials Science, Montanuniversität Leoben, Leoben, 8700, Austria — ³Microstructure and Properties of Materials (IEK-2), Forschungszentrum Jülich, 52425, Jülich, Germany

Focused ion beam (FIB) milling has been widely used to prepare micron-sized specimens for micromechanical testing, but there are different types of artefacts originated from FIB. One is the imperfections in through-thickness notch geometries of microcantilevers. Bridge notches can overcome some of the problems by, upon loading, thin bridges fail first, creating atomically sharp natural cracks. Even though this bridge failure is widely assumed and predicted by FEM simulations, it has never been observed and quantified experimentally. This study presents the first experimental observation of cracking at the bridge notch and crack arrest before the entire through-thickness notch fails. This is possible by designing very thin bridges and using

a very stiff loading rig with superior load resolution. Consequently, we obtained multiple fracture toughness values from one test. Using reported geometry correction factors calculated by FEM simulations, the fracture toughness estimated from the bridge failure was corrected and compared with the one from the failure of the through-thickness notch. The two approaches show consistent results.

MM 4.7 Mon 12:45 SCH A 216

Stable fracture of ceramics in the TEM — ORIOL GAVALDA-DIAZ^{1,2}, SHELLY CONROY¹, EDUARDO SAIZ¹, and ●FINN GIULIANI¹ — ¹Department of Materials, Imperial College London, UK — ²Department of Mechanical, Manufacturing and Materials Engineering, University of Nottingham, UK

Small scale fracture tests have allowed many elements of a microstructure to be tested in isolation such as phase or grain boundaries. In our previous work we have shown that stable fracture tests in the SEM can accurately measure surface energies and the energy of individual grain boundaries. Furthermore, these tests allow the crack path and the effect of crack-defect interactions to be studied. However, tests in the SEM struggle to give in-depth information around the crack tip. Therefore, in this work we will demonstrate how it is possible to carry out stable fracture experiments in the TEM via a double cantilever geometry. This will be demonstrated on both silicon carbide and zirconia samples where the different mechanisms of energy dissipation will be discussed. Furthermore, a stable geometry allows additional analysis to be carried out during the test, here we will discuss the possibility of using 4D STEM to map the strain field around the crack tip.

MM 5: Materials in Energy Conversion: Mechanical Properties and Solid State Batteries

Time: Monday 10:15–13:00

Location: SCH A 215

MM 5.1 Mon 10:15 SCH A 215

Interplay between mechanics and electrochemistry in Li-Si anodes by atomistic simulation — ●DANIEL MUTTER¹, MANISHA POUDEL^{1,2}, DANIEL PFALZGRAF¹, and LEONHARD MAYRHOFER¹ — ¹Fraunhofer IWM, 79108 Freiburg — ²Institute of Physics, University of Freiburg, 79104 Freiburg

Silicon is a promising anode material for Li-ion batteries due to its high capacity, which considerably exceeds that of commonly used graphite. Its direct applicability however is hampered by the huge volume change the material undergoes during loading and unloading with Li, concomitant with mechanical stresses arising in the microstructure. In this work, we provide a deeper understanding on the interplay of mechanics and electrochemistry by analyzing the effect of deformation on the electrochemical potential. Using atomistic first principles calculations, we studied crystalline as well as amorphous Li-Si phases with different Li concentrations. We present results of elastic moduli, and the change of voltage during charging and discharging cycles under various characteristic mechanical loading scenarios. The results are essential input for continuum models acting on the nanoparticle scale to correctly describe the microstructural evolution.

MM 5.2 Mon 10:30 SCH A 215

Design of zero strain cathode materials based on colquiriite-type $\text{Li}_x\text{Ca}(\text{M},\text{M}')\text{F}_6$ — ●ALJOSCHA FELIX BAUMANN^{1,2}, DANIEL MUTTER², DANIEL URBAN^{1,2}, and CHRISTIAN ELSÄSSER^{1,2} — ¹Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg im Breisgau — ²Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg

The long-term stability of Li ion batteries can be negatively affected by mechanical stresses in the microstructure of the cathode material during charge/discharge cycles. Therefore, materials are of great interest which show a zero-strain (ZS) behavior, i.e. a negligible volume change during insertion or extraction of Li ions. For specific compounds of the material class of colquiriites, $\text{Li}_x\text{A}^{\text{II}}\text{M}^{\text{III}}\text{F}_6$, ZS behavior was predicted theoretically and measured experimentally for different Li concentration ranges. In this work we investigate the effect of the electrochemically active cation M^{III} ($\text{M} = \text{Ti}, \text{V}, \text{Cr}, \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}$) on the volume change during (de-)lithiation. Using density-functional theory we calculated the equilibrium volumes at different Li concentrations. The analysis of the electronic and magnetic structures and the calculation of local structural parameters indicate that the total vol-

ume change depends mainly on the counteracting effects of expanding fluorine octahedra around the M ions due to the changing oxidation state, and a decrease of repulsion between fluorine anions due to the inserted Li ions. The trends in the properties along the period of the 3d transition metals provide a guideline for a design of new ZS cathode materials in solid solutions of type $\text{Li}_x\text{Ca}(\text{M},\text{M}')\text{F}_6$.

MM 5.3 Mon 10:45 SCH A 215

Planar gliding and vacancy condensation: The role of dislocations in the chemomechanical degradation of layered transition metal oxides — ●MARCEL SADOWSKI¹, KARSTEN ALBE¹, and SABRINA SICOLO² — ¹Technical University of Darmstadt, Darmstadt, Germany — ²BASF SE, Ludwigshafen, Germany

Stacking faults driven by dislocations have been observed in layered transition metal oxides cathodes both in cycled and uncycled materials. The reversibility of stacking-sequence changes directly impacts the material performance. Irreversible glide due to lattice invariance or local compositional changes can initiate a catastrophic sequence of degradation mechanisms. In this study we compare the chemomechanical properties of LiCoO_2 and LiNiO_2 by combining density functional theory (DFT) and anisotropic linear elasticity theory. We calculate stacking fault energies as a function of Li content and quantify the “pillar effect” of excess Ni in hindering stacking-sequence changes. We then characterize screw dislocations, which mediate stacking-sequence changes, and find a peculiarly compliant behavior of LiNiO_2 due to the interaction of Jahn-Teller distortions with the dislocation strain field. Finally, we analyze the tendency of vacancies to segregate along dislocation lines. This study represents the first instance of explicit ab-initio atomistic dislocation models in layered oxides and paves the way for the understanding and optimization of the chemomechanical behavior of cathode active materials during battery operation.

MM 5.4 Mon 11:00 SCH A 215

Modification of iron-based oxide anodes for potassium ion storage — ●ZIDONG WANG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to the abundance of potassium and its easy accessibility, potassium-based electrochemical energy storage technology has attracted extensive research interests and significant progress of it has been made in recent years. Among different anode materials for anodes of potassium-ion storage devices, transition metal oxides especially of

iron-based oxides have high potential due to their high capacity and low cost. However, their poor electrical conductivity and weak structure impede their development. In this work, adjustment of the anionic and cationic composition of iron oxides is achieved. This adjustment can effectively result in a high-performance anode for potassium ion storage. In brief, the synergistic effect of multivalent metal cations will result in excellent potassium storage properties. And the conductivity can be further improved by the replacement of anions. Our results indicate that the adjusted iron-based compound can be used as a promising high-performance anode material for potassium ion storage devices.

MM 5.5 Mon 11:15 SCH A 215

Construction of V5S8/Sb2S3@C Heterostructures as High-Performance Anode Materials for Potassium-ion Batteries

— •VINCENT HARTMANN, YULIAN DONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Transition metal sulfides (TMSs) have been studied widely and deeply as anode materials for potassium ion batteries (PIBs) owing to their relatively high theoretical capacities. However, poor electrical conductivity, large volume expansion, and slow diffusion kinetics hinder their further applications. Herein, a unique hierarchical structure of V5S8/Sb2S3@C is fabricated by a concise solvothermal method and subsequently annealing. Such a well-designed architecture affords fast K⁺ diffusion kinetics and improved charge transfer at the heterointerfaces due to the metallicity of the internal V5S8. In addition, the synergistic coupling interaction among the interior V5S8, interlayer Sb2S3, and external C layer generates a stable nanostructure, which extremely accelerates the electronic/ion transport and effectively alleviates the volume expansion upon long cyclic performance. As a result, it exhibits a high initial capacity of 525.19 mAh/g at 100 mA/g and excellent cyclic stability with 95% capacity retention after 500 cycles at 1 A/g. Our results reveal that the combination of heterostructures construction and interfacial interaction enables optimizing electronic structures and macroscopic mechanical properties of TMSs, thus achieving high-performance anodes for PIBs with high energy density.

15 min. break

MM 5.6 Mon 11:45 SCH A 215

Influence of interstitial Li on the electronic properties of Li_xCsPbI₃ for photovoltaic and battery applications

— •WEI WEI^{1,2}, 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

The stability of crystalline CsPbI₃ with interstitial Li ions is investigated together with the effect that Li has on the electronic structure of the resulting compound Li_xCsPbI₃. We analyze this by two structural models for CsPbI₃ at room temperature, the cubic α phase and a distorted structure analogous to the γ phase (γ' structure). The hypothetical α phase does thermodynamically not allow Li uptake and is likely to be structurally unstable for $x > 1/4$, while adding Li up to $x=1$ in the γ' structure is possible. In all cases, Li promotes structural distortions, namely tilting of bond angles $\Delta_{\text{Pb-I-Pb}}$ and Cs off-center displacements Δ_{rCs} , which are increasing with the Li concentration.

Interstitial Li has the following effects on the electronic structure of CsPbI₃: i) the induced structural distortion leads to a significant increase of the band gap; ii) the screening of additional electrons in the conduction band leads to a small increase of the band gap; iii) the effect of Li 2s states on the band edges and band gap is negligible. Altogether, the change of the band gap is dominated by the tilting of $\Delta_{\text{Pb-I-Pb}}$ angles: stronger distortion caused by increasing Li content is accompanied by an increased band gap.

MM 5.7 Mon 12:00 SCH A 215

Design for Dual-Functional Electrode Promoting Dendrite-free and CO₂ Utilization Enabled High-Reversible Symmetrical Na-CO₂ batteries

— •CHANGFAN XU, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

A one stone two-birds strategy is presented by using carbon paper embedded with Ru nanoparticles (RuCP) as dual-functional electrodes

for both the Na anode and CO₂ cathode. As an anode host, the RuCP with remarkable sodiophilicity can dominate Na nucleation behavior and achieve a uniform Na ion flux for the inhibition of dendrite formation, meanwhile, the RuCP affords high catalytic activity for catalyzing the formation/decomposition of Na₂CO₃ in CO₂ cathode. As a result, the Na was homogeneously deposited on the RuCP anode without Na dendrite formation, showing a high Coulombic efficiency of over 99% and a long cycle lifetime, and the RuCP cathode demonstrates low overpotentials and excellent cycling stability (>300 cycles). Implementation of the RuCP@Na anode and RuCP cathode allows for the construction of a symmetrical Na-CO₂ battery with long-duration cyclability because of the dendrite-free sodium morphology and numerous Ru catalytic sites. Such electrodes and battery designs offer an effective method for the tailoring and optimization of sodium metal batteries with high energy density.

MM 5.8 Mon 12:15 SCH A 215

Dynamic stability and *ab initio* free energy calculations of argyrodite Li₆PS₅Cl solid electrolyte

— •YONGLIANG OU, YUJI IKEDA, PRASHANTH SRINIVASAN, and BLAZEJ GRABOWSKI — Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

High ionic conductivity of argyrodite Li₆PS₅Cl, which was shown in both experiments and simulations, renders it a promising candidate for the solid electrolyte in all-solid-state lithium-ion batteries. Although the diffusion mechanism has been intensively investigated in previous studies, the dynamic and thermodynamic stability of Li₆PS₅Cl have not yet been fully understood. To address this issue, systematic investigations are carried out under the *ab initio* framework in this study. At 0 K, the dynamic instability of the ideal structure is revealed by the calculated imaginary phonon modes. Molecular dynamics simulations accelerated by machine-learning interatomic potentials show dynamic stabilization via vibrational entropy at finite temperatures. Further, *ab initio* free energy calculations are performed in wide temperature and pressure ranges utilizing a multistage thermodynamic integration technique. The calculated free energies provide important information for subsequent studies focusing on the energetic aspects, e.g., defect or grain boundary formation energy, of Li₆PS₅Cl. It can be expected that the present results benefit the research and application of all-solid-state lithium-ion batteries.

MM 5.9 Mon 12:30 SCH A 215

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 all solid-state electrolytes (SSE) known to date but their instability towards high-performance electrodes remains a critical challenge. To address this issue, we investigate the concept of rare earth lithium halides as a material-efficient, nanometer thick cathode coating in contact with thiophosphate electrolytes. Halides provide wide electrochemical stability windows as well as good chemical and thermodynamic stability [1,2].

To determine a suitable halide/thiophosphate combination, an energetically feasible reaction pathway in the multidimensional phase diagram between the two materials needs to be identified. Consequently, the thermodynamic stabilities of the emerging SSE / halide interfaces are examined by *ab initio* thermodynamics to screen reaction free enthalpies of possible interface reactions. Next, an end member analysis is performed to analyze possible compositions of interface products and possible secondary phases.

[1] J. Liang et al., Acc. Chem. Res. 2021, 54, 1023-1033 [2] K. Kim et al., Chem. Mater. 2021, 33, 10, 3669-3677

MM 5.10 Mon 12:45 SCH A 215

Active Site Deactivation of the Air Electrode in High-Temperature Solid Oxide Cells

— •HANNA TÜRK, THOMAS GÖTSCH, FRANZ-PHILIPP SCHMIDT, AXEL KNOP-GERICKE, ROBERT SCHLÖGL, THOMAS LUNKENBEIN, KARSTEN REUTER, and CHRISTOPH SCHEURER — Fritz-Haber-Institut der MPG, Berlin, Germany

Degradation of the air electrode in electrolysis mode severely limits the commercial adoption of solid oxide cells (SOCs). This degradation goes hand in hand with the oxygen evolution reaction (OER) taking place at the triple-phase boundary (TPB) between the anode, the solid electrolyte, and the gas phase. Up to now, the atomistic structure of

this active catalyst region is essentially unknown, though, which prevents a detailed analysis of the actual degradation mechanisms.

Recently, we took the first step in elucidating the TPB structure by revealing a complexation at the underlying solid/solid interface of the sintered anode[1], featuring partial amorphization and varying elemental distributions deviating from the confining bulk phases. Based on this finding, we now expand our force field based Monte-Carlo simulations

to the OER active site. Our experimentally validated results show unexpected compositional changes with respect to the thermodynamic equilibrium, that combined with a spatially resolved diffusion study indicate a hitherto unknown mechanism underlying the deactivation of the anode[2].

- [1] H. Türk *et al.*, Adv. Mater. Interfaces 8, 2100967 (2021).
 [2] H. Türk *et al.*, ChemCatChem 14, e202200300 (2022).

MM 6: Transport in Materials: Ion, Charge and Heat Transport

Time: Monday 10:15–13:00

Location: SCH A 118

MM 6.1 Mon 10:15 SCH A 118

Large-scale Atomistic and Quantum Mechanical Study of the Na⁺ Transport Mechanism in Sodium-ion Battery Electrolytes — •AMAL KANTA GIRI¹ and HARALD OBERHOFER^{1,2} — ¹University of Bayreuth — ²TU Munich

A steady increase of the greener and safer energy sources have led to a rise in the need for energy storage technologies. In the last three decades, the lithium ion batteries (LIBs) dominated the global market from small to large scale storage of the energy. Yet, the shortage of the lithium and its localized geographical distribution raises concerns. New charge carriers for batteries beyond the lithium such as Na, is viable alternative for safe and large-scale energy storage, mainly due to its large abundance and high electrochemical potential.

Here, to improve our understanding of the Na⁺ transport mechanism, aggregation, and electrolyte performance in sodium ion batteries, we perform a theoretical investigation using a combination of all-atoms molecular dynamics (MD) simulations based on the OPLS forcefield and density functional theory calculations (DFT). In this regard, we simulate NaPF₆ salt in various organic electrolytes including ethylene carbonate (EC), propylene carbonate (PC), dimethoxyethane (DME), and dimethyl carbonate (DMC), and their binary mixtures at 320 K. Specifically, we focus on the conductivity, diffusivity and solvation of Na⁺ in the liquid electrolyte mediums. Furthermore, the solvation structure and the binding energy of ions in the electrolytes are thoroughly analyzed. We find the diffusivity of Na⁺ ions in the order DMC>DME>EC>PC, which follow the viscosity of the electrolytes.

MM 6.2 Mon 10:30 SCH A 118

Fast ion conduction in glassy and crystalline phases of Na₃PS₄: Insight from a machine-learning potential molecular dynamics study — •YU-TAO LI, TABEA HUSS, CARSTEN STAACKE, KARSTEN REUTER, and CHRISTOPH SCHEURER — Fritz-Haber-Institute of the Max-Planck-Society

Its earth-abundance and chemical similarity makes sodium a promising substitute for lithium in future, sustainable solid-state batteries. In that respect the sodium thiophosphate (NaPS) material class has proven to provide electrolytes with high ionic conductivities [1]. Similar to the lithium thiophosphate (LiPS) material class, the NaPS class is characterized by a high degree of structural variety. It limits the transferability of *ab initio* studies, which are restricted to small model systems or short time scales for more complex models. Machine learning force-fields (ML-FF) provide a computationally cheaper yet sufficiently accurate alternative.

We have previously reported on a universal ML-FF for the whole LiPS material class [2]. In this work, we now develop a related ML-FF for glassy and crystalline phases of Na₃PS₄. Using the obtained ML-FF, we probe sodium ion conductivity in the glassy and crystalline phases. We systematically compare ion conductivity in LiPS vs. NaPS, and disentangle cation and anion dynamics in both material classes. Our aim is to understand the influence of stoichiometry and thiophosphate microchemistry on phase stability and ion conductivity.

- [1] A. Hayashi *et al.*, J. Power Sources 258, 420 (2014).
 [2] C.G. Staacke *et al.*, Nanomaterials 12, 2950 (2022).

MM 6.3 Mon 10:45 SCH A 118

Accelerating structure prediction of solid-solid interfaces in solid electrolytes using Machine Learning Potentials — •TABEA HUSS, CARSTEN STAACKE, 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 structural disorder and occur in a multitude of glassy and crystalline phases, depending on their stoichiometry. The most performant glass-ceramic SSEs from the LPS class are characterized by omnipresent two-dimensional interfaces between crystalline and glassy domains, which can dominate the materials performance and cycle stability. To address this complexity we present a protocol for the construction of polycrystalline solid-solid interfaces in the LPS system. Within our protocol, expensive *ab-initio* random structure search (AIRSS) calculations are replaced by a Machine Learning surrogate accelerated approach. We present a pathway towards a full assessment of partially amorphous interfaces in the LPS material class.

MM 6.4 Mon 11:00 SCH A 118

Understanding Oxide Ion Transport In Yttria Stabilized Zirconia: Fresh Insights from Molecular Dynamics Simulations — •SUDESHNA MADHUAL, KRISHNANJAN PRAMANIK, and PADMA KUMAR PADMANABHAN — Indian Institute of Technology Guwahati, Guwahati, Assam, India, 781039

A comprehensive molecular dynamics investigation of yttria stabilized zirconia, Y_xZr_{1-x}O_{2x/2}, is carried out for a wide range of compositions, x = 4 to 40 mol%, and over temperatures spanning 800 - 2200 K. The lattice parameter of the fluorite cell shows a monotonic increase with concentration, while the self-diffusivity of oxide ion as well as the resulting ionic conductivity, shows an optimum value around x = 10 mol%. These gross structural and transport properties of the system from the present study is in good agreement with previous experimental and theoretical investigations. It is noted that the oxygen migration occurs along straight channels parallel to the crystallographic axes, connecting the tetrahedral holes of the fluorite lattice occupied by them. A microscopic investigation of distinct oxygen environments, variably coordinated to Y³⁺ and Zr⁴⁺ cations, and of the channels connecting them is carried out. Analysis of these local channels for their energetics and their contribution to overall oxygen transport, resolved in terms of the cationic edges connecting them, provides fresh insights on the oxygen migration mechanism in the system.

MM 6.5 Mon 11:15 SCH A 118

Modelling accelerated ion transport in porous metal organic frameworks — •THOMAS BERGLER^{1,2} and HARALD OBERHOFER^{1,2} — ¹University of Bayreuth — ²Bavarian Center for Battery Technologies

To date, metal organic frameworks (MOFs) have found a number of successful applications, for example in gas storage or as a filter for gas mixtures. So far, these mostly incorporated them as passive materials, but recent research points the way towards a more active role, possibly through the external manipulation of the materials's internal properties. One recent example for such a property is the susceptibility of the lattice parameters of multiple specific MOFs towards electric fields, which have been shown to distort on application of the fields. The aim of this project is to further investigate this behaviour from a theoretical point of view and gain insight into it through the use of molecular dynamics (MD) and meta-dynamics (MTD) simulations. These simulations are based on density functional theory (DFT) with the Perdew-Burke-Ernzerhof (PBE) functional but also on extended tight-binding (xTB) models and MOF-specialized force-fields. After confirmation that xTB-DFT and force-field MDs yield similar results to PBE-DFT MDs, MTDs have been performed with xTB-DFT to gain information on the energy-barriers for linker rotations inside some MOFs. Afterwards, MDs of multiple ps-length and an applied external E-field were performed with these force-fields to find the minimum strength of the E-field required to have an influence on the linker's rotation statistics.

15 min. break

MM 6.6 Mon 11:45 SCH A 118

Opposite in-plane anisotropy in thermal diffusivity and resistivity — •FEI SUN¹, SIMLI MISHRA¹, PHILIPPA MCGUINNESS¹, ZUZANNA FILIPIAK¹, IGOR MARKOVIC¹, DMITRY SOKOLOV¹, SEAN HARTNOLL², ANDREW MACKENZIE^{1,3}, and VERONIKA SUNKO⁴ — ¹MPI, CPFS, Dresden, Germany — ²Univ. of Cambridge, Cambridge, UK — ³Univ. of St Andrews, St Andrews, UK — ⁴UC Berkeley, California, USA

We report the temperature dependence of the anisotropic thermal and electrical transport in the orthorhombic bilayer ruthenate Ca₃Ru₂O₇. Measurements are performed using two bespoke experimental techniques: optical measurement of thermal diffusivity, and resistivity measurements on devices micro-structured using Focused Ion Beam (FIB) sculpting. Intriguingly, we find that the electrical conductivity is higher along the direction where thermal conductivity is lower at all temperatures. The mechanism underlying this unusual behavior will be discussed in this talk.

MM 6.7 Mon 12:00 SCH A 118

Non-local microwave electrodynamic in ultra-pure PdCoO₂ — •GRAHAM BAKER¹, TIMOTHY W BRANCH¹, JAKE BOBOWSKI¹, JAMES DAY¹, DAVIDE VALENTINIS², MOHAMED OUDAH¹, PHILIPPA MCGUINNESS³, SEUNGHYUN KHIM³, PIOTR SURÓWKA⁴, YOSHITERU MAENO⁵, RODERICH MOESSNER⁶, JÖRG SCHMALIAN², ANDREW MACKENZIE³, and DOUG BONN¹ — ¹University of British Columbia — ²Karlsruhe Institute of Technology — ³Max Planck Institute for Chemical Physics of Solids — ⁴Wrocław University of Science and Technology — ⁵Kyoto University — ⁶Max Planck Institute for the Physics of Complex Systems

There has been significant recent interest in unconventional electronic transport regimes in which a local, Ohmic relationship between electric current and field breaks down. To date, the vast majority of experimental work has been done in the DC limit. Here we introduce a novel approach via AC measurements with a bespoke microwave spectrometer, using the skin effect rather than sample dimensions to induce non-local transport. Through measurements on Sr₂RuO₄ and Sn, we verify the predictions for the magnitude and frequency dependence of the surface resistance for the classical and anomalous skin effects. Data from PdCoO₂, in contrast, deviate from any previous prediction of frequency-dependent surface resistance. Analysis of such data required the construction of a more complete electrodynamic theory of metals than previously existed, and allows us to conclude that the PdCoO₂ data are due to the combination of a highly anisotropic Fermi surface and a contribution from momentum-conserving scattering.

MM 6.8 Mon 12:15 SCH A 118

Spin Hall effect in tungsten and tantalum via first-principles calculations — •REENA GUPTA, STEFANO SANVITO, and ANDREA DROGHETTI — School of Physics and CRANN, Trinity College, 2, Dublin, Ireland

We study theoretically the spin Hall effect (SHE), a phenomenon where a longitudinal charge current in a material sample gets converted into a transverse spin current and leads to spin accumulation on the sample boundaries. The common theoretical methods to calculate the intrinsic SHE conversion efficiency (i.e., the "spin Hall angle") are semi-classical or rely on the relaxation time approximation. To go beyond these lim-

itations, we combine the non-equilibrium Green's function approach with Density Functional Theory. We study the SHE in bulk as well as slab geometries for different phases of tungsten and tantalum. We find values for the spin Hall angles, which are comparable to the most recent experimental results. Furthermore, in the slab geometries, we find that the spin Hall effect is accompanied by current-induced spin polarization (CISP). We then discuss the relative magnitude of the SHE and of CISP suggesting how the two effects can be distinguished in experiments.

MM 6.9 Mon 12:30 SCH A 118

Transport properties of Dirac materials: the role of plasmons — •KITINAN PONGSANGANGAN — TU Dresden, Dresden, Germany

We study the thermoelectric transport of Coulomb interacting Dirac electrons with Keldysh quantum field theory. We study it from a weak-coupling and a strong-coupling perspective. We demonstrate that long-range Coulomb interactions play two independent roles: (i) they provide the inelastic and momentum-conserving scattering mechanism that leads to fast local equilibration; (ii) they facilitate the emergence of collective excitations, for instance plasmons, that contribute to transport properties on equal footing with electrons. Our approach is based on an effective field theory of the collective field coupled to electrons. Within a conserving approximation for the coupled system we derive a set of coupled quantum-kinetic equations. This builds the foundation of the derivation of the Boltzmann equations for the interacting system of electrons and plasmons. From this, we explicitly derive all the conservation laws and identify the extra contributions of energy density and pressure from the plasmons. We demonstrate that plasmons show up in thermo-electric transport properties as well as in quantities that enter the energy-momentum tensor, such as the viscosity.

MM 6.10 Mon 12:45 SCH A 118

Dragging effect of the Berry curvature in ferromagnetic Weyl semimetals NiMnSb and PtMnSb — SUKRITI SINGH¹, •ANA GARCÍA-PAGE¹, JONATHAN NOKY¹, SUBHAJIT ROYCHOWDHURY¹, MAIA G. VERGNIORY^{1,2}, HORST BORRMANN¹, HANS-HENNING KLAUSS³, CLAUDIA FELSER¹, and CHANDRA SHEKHAR¹ — ¹Max-Planck-Institute for Chemical Physics of Solids, Dresden 01187, Germany — ²Donostia International Physics Center, Donostia-San Sebastián 20018, Spain — ³Institute for Solid State and Materials Physics, Technische Universität Dresden, Dresden 01069, Germany

The Anomalous Hall effect is a transport phenomenon in ferromagnets, which exhibit currents even in the absence of a magnetic field. Their inner magnetization breaks Time Reversal Symmetry, allowing the Berry Curvature (BC) to be finite. As a result, topological features close to the Fermi energy have a deep impact in the transport properties, leading to huge Anomalous Hall Conductivities (AHC). This has been a well-established paradigm for the last years for the linear AHC.

However, recent experimental results in the Weyl semimetals NiMnSb and PtMnSb might be pointing to something beyond it. By combining ab-initio calculations with a toy-model, we show that the steep slope-bands both compounds exhibit are capable of dragging the BC originated in Weyl nodes far away from the Fermi level, leading to a huge AHC in these compounds. We propose that this dragging effect of the BC can be generalized to the other materials exhibiting this band structure behaviour, which enriches the paradigm described above. Further research in this direction is currently being done.

MM 7: Invited Talk: Merkert

Time: Monday 15:00–15:30

Location: SCH A 251

Invited Talk MM 7.1 Mon 15:00 SCH A 251
Molecular dynamics simulations of shock waves in alloys: Interplay of defects and phase transition — ●NINA MERKERT — TU Clausthal, Germany

The study of materials under high-pressure conditions is essential not only for industrial activities but also for geological and astronomical applications. We consider iron and iron-carbon alloys showing a pressure induced phase transformation from the bcc to the hexagonal close-packed phase at around 13 GPa depending on the carbon content. We study compression waves in polycrystalline Fe and Fe-C using interatomic potentials that faithfully incorporate this phase transition

at the desired equilibrium pressure.

Our simulations show that the phase transformation is preceded by plastic activity, leading to the so-called 3-wave structure: An elastic compression wave is followed by a plastic wave, which then leads to a phase-transformation front. We investigate the interplay of defects in bcc with the transformation process. These defects also influence the fracture (spallation) of the shocked iron samples.

Recently, we extended our results to high-entropy alloys (HEAs) that consist of equiatomic mixtures of five or more elements and are attracting increasing interest due to their promising material properties. We studied shock-induced spallation in HEAs and found exceptionally high spall strengths that are beneficial for high strain-rate applications.

MM 8: Development of Computational Methods: Diverse Topics and Machine Learning

Time: Monday 15:45–17:45

Location: SCH A 251

MM 8.1 Mon 15:45 SCH A 251
Adaptively Compressed Exchange in LAPW — ●DAVIS ZAVICKIS, KRISTIAN KACARS, JANIS CIMURS, and ANDRIS GULANS — Electronic Structure Group, University of Latvia, Jelgavas st. 3, LV-1004, Riga, Latvia

We address precision and reproducibility issues in DFT calculations with hybrid functionals. Linearized augmented plane waves (LAPW) method currently serves as the de facto reference tool within the electronic structure community. In the current implementation of the Fock exchange in LAPW, the total and band energies depend on the number of orbitals used. We overcome these issues by implementing the adaptively compressed exchange (ACE) method [Lin Lin, J. Chem. Comput., 2016, 12, 5] in `exciting` code that introduces a low rank approximation and apply it to light atoms, molecules and solids [D. Zavickis et al., Phys. Rev. B., 2022, 106, 165101]. In case of atoms and molecules, we show that ACE leads to highly precise total energies which are within a few microhartrees off the results obtained by multi-resolution analysis method. In solids we calculate band structures that are compared with other all-electron hybrid implementations. Lastly, we apply optimizations and fine tuning to ACE, analyze its complexity and computational performance by comparing it to the previous Fock-exchange implementation in the `exciting` code.

MM 8.2 Mon 16:00 SCH A 251
How much laser power can two-photon 3D printed microoptics withstand? — ●SEBASTIAN KLEIN, PAVEL RUCHKA, TOBIAS STEINLE, and HARALD GIESSEN — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

In recent years, the manufacturing of small 3D printed microoptics has seen a rise in importance. 3D printed lenses are used for applications where space is of big concern. Tailored free form optics are ideally suited to improve the performance for specific use cases. New applications also include printing these optics onto optical fibers, for example for endoscopes in the biomedical field or for focusing a laser beam inside a compact fiber laser. In the latter case, the sustainability of high intensities of the pump laser is important. This is directly dependent on the maximum power the material of the lens can withstand.

In this work, we obtain a first insight into laser damage thresholds of the 2PP photoresist IP-S in the near-IR spectral range. We determine damage thresholds with femtosecond laser pulses for wavelengths in the range of 1550-2000 nm. We conduct these experiments on cube samples printed from IP-S and evaluate the damage of the exposed samples visually under a microscope, employing also differential interference contrast. The observed damage is mostly of thermal nature. Knowledge of damage thresholds of 3D printed micro-optics further pushes the applications to these limits, enabling high-power applications at safe operating intensities.

MM 8.3 Mon 16:15 SCH A 251
Molecular Dynamics Simulation of Selective Laser Melting — FABIO OELSCHLÄGER¹, AZAD GORGIS¹, DOMINIC KLEIN¹, SARAH MÜLLER², and ●JOHANNES ROTH¹ — ¹FMQ, Universität Stuttgart, Germany — ²GSaME, Universität Stuttgart, Germany

Traditionally, manufacturing has been subtractive which means removing material from a workpiece. Additive manufacturing on the other hand is defined by successive addition of material and fusion with the help of heat for example. Here we report atomistic simulations of selective laser melting (SLM) used to produce additive manufactured objects. After a short introduction into the subject we present challenges to SLM. Next, modifications to basic molecular dynamics simulation are described which are required to simulate the annealing process. Although the sample sizes studied are already impressively large, scaling of system parameters are required to relate simulation and experiment. First results from the study of single and rows of spheres will be reported and further developments and improvements will be addressed.

MM 8.4 Mon 16:30 SCH A 251
Exploring Enhanced Sampling Concepts based on Boltzmann Generators — ●DAVID GRETEN, KARSTEN REUTER, and JOHANNES T. MARGRAF — FHI Theory Department, Berlin, DE

Computational surface science and catalysis research is still mainly conducted with static density functional theory (DFT) calculations. This approach is computationally convenient, but misses important aspects of surface chemistry, such as anharmonic free energy contributions. In principle, DFT-based molecular dynamics (MD) simulations (ideally combined with enhanced sampling algorithms) would allow a much more accurate description of these processes. Unfortunately, these are far too expensive to be routinely applied to complex surface/adsorbate systems. This is due to the fact that configurations in MD are generated sequentially. As a consequence, MD configurations are not statistically independent so that a very large number of samples is required to obtain converged ensemble properties. To overcome this limitation, Noé and co-workers recently proposed a generative machine learning model called the Boltzmann Generator, which was used to generate independent configurations of biomolecules. In this contribution, we explore how we can expand ML based sampling concepts utilizing Boltzmann Generators. In particular, training protocols and validation metrics will be discussed.

15 min. break

MM 8.5 Mon 17:00 SCH A 251
When does the Tamura model of phonon-isotope scattering break down? — ●NAKIB PROTİK and CLAUDIA DRAXL — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

A standard approach to the phonon-isotope scattering problem is the Tamura model [1]. This non-self-consistent 1st Born approximation of the scattering T-matrix expansion is exact for the low energy phonons, and higher order perturbative corrections for the higher energy, dispersive acoustic phonons have been argued to be small [1]. To our knowledge, the validity of this approach for the optic phonons has not yet been demonstrated. In this talk, we compare the Tamura model to the ab initio computed non-perturbative phonon-isotope scattering T-matrix for a set of well-studied materials. We show under what

conditions the Tamura model breaks down.

[1] Tamura, S. I. (1983). Isotope scattering of dispersive phonons in Ge. *Physical Review B*, 27(2), 858.

MM 8.6 Mon 17:15 SCH A 251

Physics-inspired Machine Learning for Predicting Ionization Energies of Electronically Localized Systems — ●KE CHEN^{1,2,3}, CHRISTIAN KUNKEL¹, BINGQING CHENG³, KARSTEN REUTER¹, and JOHANNES T. MARGRAF¹ — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²Technische Universität München, Garching, Germany — ³Institute of Science and Technology, Klosterneuburg, Austria

Machine learning (ML) has been successfully applied to predict many chemical properties, most prominently energies and forces in molecules and materials. The strong interest in predicting energies in particular has led to a 'local energy'-based paradigm for modern chemical ML models, which ensures size extensivity and linear scaling of computational cost. However, some electronic properties (such as excitation energies or ionization potentials) are not size-extensive and may even be spatially localized. Using extensive models in these cases can lead to large errors. In this work, we explore different strategies for predicting intensive and localized properties, using ionization energies in organic molecules as a test case. In particular, we compare size-intensive aggregation functions and effective, machine-learned Hamiltonians. The physical interpretability and cost/benefit ratios of the approaches will

be discussed.

MM 8.7 Mon 17:30 SCH A 251

Kernel Charge Equilibration: Machine Learned Interatomic Potentials With Full Long-Range Electrostatics — ●MARTIN VONDRAK, JOHANNES T. MARGRAF, and KARSTEN REUTER — Fritz Haber Institute of the Max Planck Society, 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 mapping between a systems structure its physical properties. State-of-the-art models typically represent chemical structures in terms of local atomic environments to this end. This inevitably leads to the neglect of long-range interactions (most prominently electrostatics) and non-local phenomena (e.g. charge transfer), resulting in 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. In this contributions, strategies for creating kQEq interatomic potentials are discussed, including the combination of short-ranged Gaussian Approximation Potentials with kQEq.

MM 9: Topical Session: Fundamentals of Fracture – Interface Fracture

Time: Monday 15:45–18:00

Location: SCH A 216

Topical Talk

MM 9.1 Mon 15:45 SCH A 216

Modeling of grain boundary embrittlement phenomena in metallic materials — ●LORENZ ROMANER¹, ALEXANDER REICHMANN¹, CHRISTOPH DÖSINGER¹, TOBIAS SPITALER¹, DANIEL SCHEIBER², OLEG PEIL², MARKUS ALFREIDER¹, MICHAEL WURMSHUBER¹, and DANIEL KIENER¹ — ¹Department of Materials Science, Montanuniversität Leoben, 8700 Leoben, Austria. — ²Materials Center Leoben Forschung GmbH, 8700 Leoben Austria.

Intergranular embrittlement phenomena are of strong relevance for many technological materials including steels, nickel-based alloys, coinage metals or refractory metals. The decisive process is grain boundary segregation where solutes diffuse and enrich at grain boundaries thereby modifying their cohesive properties which can favor or impede crack propagation. We present a multi-scale simulation framework for grain boundary segregation employing atomistic, thermokinetic and data-driven computational methods and show how chemistry and propensity against crack propagation can be modeled from basic knowledge of composition and processing parameters. Validation examples with several experimental methods including atom probe tomography, high resolution transmission electron microscopy and micro-mechanical testing are presented. Furthermore, we discuss the potential of statistical learning methods to replace density functional theory simulations in future, in particular to address advanced phenomena such as concentration dependence and co-segregation.

MM 9.2 Mon 16:15 SCH A 216

Atomistic study of impurity-induced intergranular embrittlement in tungsten — ●PÄR A. T. OLSSON^{1,2}, PRAVEENKUMAR HIREMATH², and SOLVEIG MELIN² — ¹Materials Science and Applied Mathematics, Malmö University, SE-205 06 Malmö, Sweden — ²Division of Mechanics, Materials & Components, Lund University, Box 118, SE-221 00 Lund, Sweden

In the present work we study the impact of phosphorus (P) impurities on the grain boundary strength of tungsten (W) by means of classical atomistic modelling to explore the role of impurities on the grain boundary (GB) embrittlement of W. To this end, we have fitted a new binary 2NN-MEAM potential for the W-P system that is designed to capture the embrittling potency of P in W GBs as predicted by means of density functional theory (DFT) modelling. Analysis of the GB work of separation and generalized stacking fault energy data derived from DFT and the 2NN-MEAM potential show that substitutional P-impurities reduce the resistance to both cleavage and slip. Mode I tensile and crack simulations reveal that the most dominant mode of GB failure is cleavage and that pristine GBs, which are initially ductile, on most accounts change to brittle upon introduction of

impurities. Such tendencies are in line with experimentally observed correlations between P-impurity content and reduced ductility.

MM 9.3 Mon 16:30 SCH A 216

Characterization of the stability of metal/metal interfaces by atomistic simulations — ●DANIEL F. URBAN, REYHANEH GHASEMIZADEH, and CHRISTIAN ELSÄSSER — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

The reliable prediction of the adhesion and mechanical stability of interfaces between two metal phases from density functional theory (DFT) calculations remains a challenge. One possible approach to systematically address this issue is an idealized cleavage simulation analysed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. Another approach is the study of the gamma surface, i.e. the generalized stacking fault energy, as function of lateral displacement, which yields information on the critical resolved shear stress of dislocation motion. Here we systematically study coherent [111]-oriented interfaces between fcc metals in terms of the above mentioned methods. We analyze the interface energy in terms of coupled tensile and shear displacements which include the effect of the tension softening of the interface. Furthermore, the influence of an additional lateral mechanical strain on the two phases, as often present in experimentally grown thin layers, is examined.

15 min. break

MM 9.4 Mon 17:00 SCH A 216

The heterogeneous nature of grain boundary segregation and embrittlement — ●REMI DINGREVILLE — Sandia National Laboratories, Albuquerque NM, USA

Nanostructured materials are inherently unstable due to the high density of non-equilibrium defects that provide a substantial driving force for exaggerated or unexpected evolution. Departing from most mesoscale models for grain boundaries (GB), there is a clear recognition that GB properties, especially GB embrittlement and GB fracture, are not single-valued for a given material, but widely disparate depending on the configuration of the particular boundary and its neighboring grain. Taking this one step further, both GB character and GB defects control the GB embrittlement and fracture in response to mechanical, thermal, and irradiation stimuli. Each different type of stimuli perturb the GB character in distinctly different processes: e.g. stress causes elastic mismatch that tilts the energy barrier whereas strain drives specific dislocation content into the GB; non-implanting irradiation on

the other hand creates local thermal spikes and atomic shuffling. In this presentation, I will discuss these effects on GB segregation and GB fracture properties from both a theoretical and atomistic perspectives.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy National Nuclear Security Administration under contract DE-NA0003525.

MM 9.5 Mon 17:15 SCH A 216

Modelling the grain boundary segregation of phosphorus in iron using thermodynamical approaches and Bayesian inference — ●ALEXANDER REICHMANN¹, CHRISTOPH DÖSINGER¹, DANIEL SCHEIBER², OLEG PEIL², VSEVOLOD RAZUMOVSKIY², and LORENZ ROMANER¹ — ¹Department of Materials Science, Montanuniversität Leoben, Austria — ²Materials Center Leoben Forschung GmbH, Leoben, Austria

The chemistry and structure of grain boundaries (GBs) play a key role for understanding fracture in metallic alloys. Atomistic simulations provide a direct access to one of the key fundamental GB characteristics, the GB solute segregation energy. Experimentally, the solute segregation can be evaluated by measuring the GB solute concentration using a variety of techniques, one of which is the Auger electron spectroscopy. However, a direct comparison of experimentally measured GB solute excess and calculated GB segregation energy requires an additional step of conversion, which is a non-trivial task in many cases. As a result, calculated and measured data are not always found in good agreement with each other and often require an in-depth investigation. In this talk, we will present an approach for getting a consistent comparison between the calculated and experimentally measured data based on the Bayesian inference framework, which we use in combination with Markov chain Monte Carlo simulations for uncertainty quantification and model evaluation. We apply this framework to analyze phosphorus segregation in iron and evaluate theoretical and experimental data on GB excess.

MM 9.6 Mon 17:30 SCH A 216

Characterizing interface toughness in functional materials — ●ELOHO OKOTETE¹, SUBIN LEE¹, STEFFEN BRINCKMANN², and CHRISTOPH KIRCHLECHNER¹ — ¹Institute for Applied Materials, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — ²Structure and Function of Materials (IEK-2), Forschungszentrum Jülich, 52425 Jülich, Germany

Interfaces are the backbones of functionality in emerging material sys-

tems for this new age. However, mechanical failure usually occurs in these interfaces leading to degradation of functional properties. Experimental methods to investigate the interface strength and its failure mechanisms include peel test, super layer test, or indentation test. These methods output qualitative data with huge experimental scatter and a lack of in-depth understanding of underlying mechanisms of failure. Small-scale mechanical testing using single and double cantilever beams makes it possible to extract quantitative data for interface properties of micro/ nanometer-sized films. However, these methods are prone to unstable crack growth, finite notch root radius, and other problems arising from testing geometries. In this talk, we propose a new micro cantilever design that provides reliable quantitative interface toughness. Our initial finite element calculations showed the optimized geometry could propagate a pre-notch in a stable manner, which is essential to generate a natural crack front without FIB-induced damage/artifacts. This observation is validated with in situ experiments on the interface between a hard coating and silicon substrate.

MM 9.7 Mon 17:45 SCH A 216

Abnormal internal oxidation of grain boundary and its cracking behavior under mechanical stress in an FeCr alloy — ●KUAN DING¹, XIAO SHEN², SIYUAN ZHANG³, JIEJIE LI⁴, ENRICO BRUDER¹, JIANJUN LI⁴, WENWEN SONG², KARSTEN DURST¹, JAMES P. BEST³, and XUFEI FANG¹ — ¹Department of Materials and Earth Sciences, TU Darmstadt, 64287 Darmstadt, Germany — ²Steel Institute (IEHK), RWTH Aachen University, 52072 Aachen, Germany — ³Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — ⁴School of Mechanical and Electrical Engineering, Central South University, 410083 Changsha, China

FeCr-based Ferritic stainless steels display great potential for applications as interconnects of solid oxide fuel cells at temperatures below 800 °C. Cr provides good oxidation resistance by forming a protective oxide layer to prevent the substrate from exposing to corrosive environment. However, grain boundaries (GBs) act as fast diffusion paths, and internal oxidation along the GB can form brittle oxide, which is prone to cracking under mechanical stresses. In this work, we investigated the abnormal growth of GB oxide at 600 °C in air and its impact on GB cracking in Fe-15wt.%Cr alloy. The microstructure and chemical characterization of the abnormal GB oxide revealed a layer of chromium oxide forming with a large penetration depth. To study the mechanical response, we conducted both ex-situ and in-situ micromechanical tests and simulation and observed the cracking behavior of the abnormal GB oxide. Our finding provides insights into improving the oxidation and fracture resistance through material design.

MM 10: Materials for Storage and Conversion of Energy: New Storage Materials

Time: Monday 15:45–16:45

Location: SCH A 215

MM 10.1 Mon 15:45 SCH A 215

Improving the cleanliness of TEM investigation of catalyst samples — ●JULIA MENTEN¹, ROBERT SCHLÖGL^{1,2}, and WALID HETABA¹ — ¹Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany — ²Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Transmission electron microscopy (TEM) offers a powerful tool for the analysis of specimens down to an atomic scale. In order to achieve high quality data, sample preparation is a crucial step. Many samples contain a high carbon content, e.g. as organic ligands or solvents. Electron beam exposure can lead to the deposition of carbon on the specimen surface and limit the image resolution and quality of obtained spectroscopic data. Different mitigation strategies can be applied in order to reduce contamination, though these methods can easily harm the specimens or lead to accumulation of carbonaceous molecules in the microscope environment [1].

In our work we focus on the removal of undesirable carbon species before the sample is inserted into the microscope. Our sample cleaning setup allows to investigate the influence of different preparation parameters, e.g. drying time or temperature, on how long solvents remain in the vacuum system and therefore can have an impact on the TEM analysis. Evaluation of the decrease in pressure while pumping our setup with a TEM sample gives insight in necessary drying times. The impact of our sample treatment can be investigated in the TEM by evaluating contrast and thickness measurements.

[1] Mitchell, Micron 73 (2015) 36-46

MM 10.2 Mon 16:00 SCH A 215

Ultrafast Electron Transfer in Photoexcited Fullerene-Derivatives — ●MOHAMED E. MADJET, ADRIAN DOMINGUEZ-CASTRO, FULU ZHENG, and THOMAS FRAUENHEIM — Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany

Fullerene derivatives continue to attract a lot of interest both experimentally and theoretically. They have been known to be excellent electron acceptors due to their interesting ground and excited state properties. The chemical functionalization of fullerenes makes possible to synthesize and develop new compounds. These derivatives are used as building blocks for molecular complexes and devices with potential applications in solar cells, sensing and in biomedical applications. Using non-adiabatic molecular dynamics simulations combined with time-dependent density functional theory [1-3], we study the photoinduced electron dynamics and charge transfer processes in some fullerene derivatives upon a selective and localized excitation on the donor molecule. Results on hot electron dynamics, charge transfer and nonradiative recombination processes will be presented, discussed, and compared to the experimental results in [4].

References

[1] Madjet et al, PRL 126, 183002(2021) [2] Smith, Shakiba and Akimov, J.Chem. Theory Comp. 17, 678 (2021). [3] Shakiba, Stippel and Akimov, J. Chem. Theory Comp., in print (2022) [4] Julio R. Pinzo

et al, J. Am. Chem. Soc. 131, 7727 (2009)

MM 10.3 Mon 16:15 SCH A 215

Carrier Multiplication in Transition Metal Dichalcogenides Beyond Threshold Limit — ●YUXIANG LIU¹, THOMAS FRAUENHEIM¹, and CHYUNG YAM² — ¹Bremen Center for Computational Materials Science, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany — ²Shenzhen Institute for Advanced Study, University of Electronic Science and Technology of China, Shenzhen, 518000, China

Carrier multiplication (CM), multiexciton generation by absorbing a single photon. Beard et al. predicted that CM could overcome the Shockley-Queisser limit and raise solar cell efficiency to ~46%[1]. The current state-of-the-art nanomaterials including quantum dots and carbon nanotubes have demonstrated CM phenomenon, but not satisfactory owing to high threshold energy and inherent difficulties with carrier extraction. We found a below threshold limit CM in monolayer transition metal dichalcogenides (TMDCs) MX₂ (M = Mo, W; X = S, Se, Te). Surprisingly, the threshold energy of CM in monolayer TMDCs can be substantially reduced due to lattice vibrations. Electron-phonon couplings (EPC) could cause significant changes in electronic structures, even trigger semiconductor-metal transition, and eventually decrease the threshold energy of CM to less than twice

bandgap[2]. Our results identify TMDCs as attractive candidate materials for efficient optoelectronic devices with the advantages of high photoconductivity and phonon-assisted tunable CM characteristics.

Reference [1] Beard, M. C., et al., Acc. Chem. Res., 46, 1252–1260(2013). [2] Yuxiang L., et al., Adv. Sci., 9, 2203400 (2022).

MM 10.4 Mon 16:30 SCH A 215

Vibronic quantum coherences in orthorhombic lead halide perovskite — ●AJAY JHA^{1,2}, ZIHUI LIU⁵, VANDANA TIWARI², PABITRA NAYAK³, HENRY SNAITH³, XIAN-TING LIANG⁵, R. J. DWAYNE MILLER⁴, and HONG-GUANG DUAN⁵ — ¹Rosalind Franklin Institute, Didcot, UK — ²MPI-Structure and Dynamics of Matter, Hamburg, Germany — ³University of Oxford, Oxford, UK — ⁴University of Toronto, Toronto, Canada — ⁵Ningbo University, Ningbo, China

To unravel the quantum coherent dynamics in orthorhombic perovskite, we employ the ultrafast two-dimensional coherent spectroscopy in methylammonium lead iodide perovskite at 15 K. The data clearly resolve the exciton and carrier band in perovskite along with the interaction between exciton and carriers by observation of cross peaks. The ultrafast population transfer from charge carriers to exciton in perovskite is associated with the vibrational coherences. The nature and role of these coherences will be discussed in detail.

MM 11: Functional Materials: Performance, Reliability and Degradation

Time: Monday 17:00–18:15

Location: SCH A 215

MM 11.1 Mon 17:00 SCH A 215

Stability and electronic structure of NV centers at dislocation cores in diamond — ●REYHANEH GHASSEMIZADEH, WOLFGANG KÖRNER, DANIEL F. URBAN, and CHRISTIAN ELSÄSSER — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Due to its outstanding coherence properties, the negatively charged nitrogen-vacancy defect (NV center) in diamond is a promising system for quantum magnetometry and solid-state based quantum computing. However, its performance can be limited by the presence of crystal defects. We study the influence of dislocations on the stability and physical properties of the NV center within a density functional theory analysis [1]. We model the most common dislocations in diamond, namely the 30° and 90° partial glide, and calculate the defect formation energy, structural geometry, electronic defect levels and zero-field splitting (ZFS) parameters. Our simulations reveal that dislocations potentially trap NV defects with an energy release of up to 3 eV. In general, the properties of NV centers at dislocations show strong deviations with respect to their bulk values. However, the lowest energy configuration of a NV center at the core of a 30° dislocation shows very bulk-like properties. Its electronic level spectrum is only slightly modified and ZFS values deviate less than 5% from their bulk values. These results open the perspective to align multiple NV centers along this dislocation type with a linear-chain arrangement whose collective behavior may become advantageous for quantum technology applications. [1] R. Ghassemizadeh et al., Phys. Rev. B 106, 174111 (2022)

MM 11.2 Mon 17:15 SCH A 215

First-principles calculation of electroacoustic properties of wurtzite (Al,Sc)N — ●DANIEL F. URBAN¹, OLIVER AMBACHER², and CHRISTIAN ELSÄSSER¹ — ¹Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — ²INATECH—Department of Sustainable Systems Engineering, University Freiburg, Germany

We study the electroacoustic properties of aluminum scandium nitride crystals Al_{1-x}Sc_xN with the metastable wurtzite structure by means of first-principles calculations based on density functional theory [1]. We extract the material property data relevant for electroacoustic device design, namely the full tensors of elastic and piezoelectric constants. Atomistic models were constructed and analyzed for a variety of Sc concentrations 0 ≤ x ≤ 50%. The functional dependence of the material properties on the scandium concentration was extracted by fitting the data obtained from an averaging procedure for different disordered atomic configurations. We give an explanation of the observed elastic softening and the extraordinary increase in piezoelectric response as a function of Sc content in terms of an element specific analysis of bond lengths and bond angles.

[1] D. F. Urban, O. Ambacher, and C. Elsässer, Phys. Rev. B 103, 115204 (2021)

MM 11.3 Mon 17:30 SCH A 215

Template-mediated well-defined nanostructure arrays for optical, electrical, and magnetic applications — ●RUI XU¹, DENYS MAKAROV¹, and YONG LEI² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Ilmenau University of Technology, Ilmenau, Germany.

Advanced devices play a critical role for sustaining the ever-growing demands of our society for energy, information, health care, etc. To achieve high performance, devices with nanoscaled features are attracting more and more attentions by virtue of their unique and promising effects emerging at nanoscale. Structural design and engineering of materials provides a versatile platform to optimize the device performance and improve the commercial competitiveness. Regarding the structural engineering, controlling the geometrical parameters (i.e., size, shape, hetero-architecture, and spatial arrangement) of nanostructures have been the central aspects of investigations and practical applications. By using anodic aluminum oxide template, we realized well-defined controlling of nanostructures over the size, in-plane/out-of-plane shape, hetero-architecture, and spatial arrangement. With such well-defined nanostructures, the optical, electrical, and magnetic performance of nanodevices can be obviously enhanced.

MM 11.4 Mon 17:45 SCH A 215

Advantages of oxygen-free wire-arc sprayed titanium coatings — ●MAIK SZAFARSKA¹, MANUEL RODRIGUEZ DIAZ², CORNELIUS BOEKHOFF¹, RENÉ GUSTUS¹, KAI MÖHWALD², HANS JÜRGEN MAIER², and WOLFGANG MAUS-FRIEDRICH¹ — ¹TU Clausthal, Clausthal Centre of Material Technology — ²Leibniz Universität Hannover, Institut für Werkstoffkunde

Typically, thermal spraying is carried out in air, with compressed air acting as the cooling agent. However, the application of oxygen-affinitive materials like titanium is heavily influenced by the oxygen content in the atmosphere. Besides the impact on chemical composition, it can negatively influence the wetting behavior of the surface, the residual stress inside the coating and the formation of cracks and defects. Alternatives like cold gas spraying and vacuum plasma spraying grant only slight improvements coupled with an increased difficulty or cost for industrial use. Using silane-doped argon, it is possible to reduce the oxygen partial pressure to extremely low levels well below 10E-23 mbar. This makes application of wire-arc spraying possible for oxygen-affinitive materials like titanium. The titanium coatings feature a significantly reduced porosity caused by improved wetting behavior of titanium particles during the spraying process. Additionally, the coatings show extremely high adhesive tensile strengths compared

to coatings formed in air. Discussed topics include particle formation, surface morphology and chemical composition, splat profiles, coating cross sections and interfacial diffusion between titanium coatings with iron-substrates.

MM 11.5 Mon 18:00 SCH A 215

Simulative study on crocheted fabrics via finite element method — ●JAN LUKAS STORCK¹, DENNIS GERBER¹, LISKA STEENBOCK¹, and YORDAN KYOSEV² — ¹Bielefeld University of Applied Sciences, Bielefeld, Germany — ²Technische Universität Dresden, Dresden, Germany

Crochet is a rarely studied but very versatile textile technology. Industrial production of crochet does not yet exist but approaches to automation have recently emerged. In order to research the properties of crocheted fabrics by simulation, the finite element method (FEM)

is well suited as a numerical approach due to the high complexity of the crochet structure. To the best of our knowledge, the FEM study presented here is the first one on the basic mechanical properties of crocheted fabrics [1]. A topology based key point model of an exemplary crocheted fabric at the meso scale was developed and studied with LS-DYNA (Livermore Software Technology Corporation). Displacements in the two textile directions (course and wale) revealed an even distribution of stresses in the fabric, whereby the stresses in course direction propagated faster. This and the differing stitch deformations show anisotropic properties. Such fast-calculating FEM simulations in combination with the developed flexible modelling can also be used in the future for engineering crocheted textiles for technical applications.

Reference [1]: J. L. Storck, D. Gerber, L. Steenbock, Y. Kyosev. Topology based modelling of crochet structures. Journal of Industrial Textiles, 2022, accepted, doi: 10.1177/15280837221139250.

MM 12: Poster I

Time: Monday 18:15–20:00

Location: P2/OG1+2

MM 12.1 Mon 18:15 P2/OG1+2

Time-of-Flight X-ray Photoelectron Microscopy (ToF-X-PEEM) — ●G. SCHÖNHENSE¹, O. TKACH^{1,2}, O. FEDCHENKO¹, Y. LYTVYENKO¹, D. VASILYEV¹, Q.L. NGUYEN³, T.R.F. PEIXOTO⁴, A. GLOSKOVSKI⁴, S. CHERNOV⁴, M. HOESCH⁴, N. WIND^{4,5}, M. HEBER⁴, C. SCHLUETER⁴, C. SHARMA⁵, K. ROSSNAGEL^{4,5}, M. SCHOLZ⁴, and H.-J. ELMERS¹ — ¹Mainz Univ. — ²Suny State Univ. — ³SLAC Nat. Accel. Lab., USA — ⁴DESY Hamburg — ⁵Kiel Univ.

The classical solution for photoelectron imaging in the X-ray range (X-PEEM) employs a hemispherical analyzer, as first described by Tonnerl. X-PEEM shows reduced spatial and energy resolution and notoriously low transmission, a consequence of the slits and small angular acceptance of the hemisphere. ToF-X-PEEM combines time-of-flight energy recording with a new lens optics minimizing spherical aberration. Systematic ray tracings predict a resolution in the (sub-) micron range, when a k-confining aperture array is placed in the second reciprocal plane, where the k-magnification can be zoomed in a large range. The new optics has been recently commissioned at PETRA-III (soft X-rays), studying ultrathin flakes and Moiré sandwich patterns of various transition-metal dichalcogenides. We demonstrate the high quality of deposited flakes by systematic ToF-X-PEEM characterization. Imaging large field of view >3mm with widened X-ray beam profile enables rapid chemical mapping with frame rates up to 1/s for strong core levels. Contracting the beam spot to <20µm and placing it on the desired flake allows small-area SX-ARPES employing the momentum-microscopy mode. [1] B.Tonner, NIMS A291, 60(1990)

MM 12.2 Mon 18:15 P2/OG1+2

Chlorine Corrosion of Superheater Steels — ●MATTHIAS KROH, SEBASTIAN PENTZ, FERDINAND HAIDER, and GEORG KRUPKOV — Univ. Augsburg, Inst. f. Physik, 86159 Augsburg

During combustion in waste-incineration-plants a variety of chemical substances are released into the gas stream. Especially under the environment present in an incineration plant the active Chlorine-catalysed high temperature corrosion caused by released Cl₂ and HCl proves detrimental to the lifetime of heat exchanger tubes, which are essential for the power production. According to literature, Cl₂ is far more corrosive than HCl, but these studies were rather qualitative and do not reflect conditions like e.g. in a real power plant. To simulate this process in a laboratory environment with realistic Cl-concentrations, a Chlorine generator was designed, which produces Cl₂ from a reaction of liquid NaOCl and H₂SO₄. The formed Chlorine concentrations were quantified via GCMS and UV VIS spectrometry to produce Cl₂ concentrations akin to those in real plants. In these experiments the corrosional attack of Cl₂ and of HCl on samples of a typical superheater steel was determined for various temperatures and defined gas atmospheres. Especially the influence of water and sulfur dioxide in the gas atmosphere were studied. The experimental setup is based on a horizontal furnace, containing the samples in a quartz tube, exposed to a flow of the desired gas atmosphere, and a subsequent gas analysis. Weight loss of the samples after removing reaction products as well as the morphology of the reaction zone are determined after various exposure times.

MM 12.3 Mon 18:15 P2/OG1+2

Nanoscale heat transport in heterostructures measured with UXRD at European XFEL — ●JAN-ETIENNE PUDELL^{1,2,3}, MARC HERZOG², MAX MATTERN², JASMIN JARECKI², ALEXANDER VON REPPERT², ULRIKE BOESENBERG¹, ANGEL RODRIGUEZ-FERNANDEZ¹, WONHIUK JO¹, ROMAN SHAYDUK¹, WEI LU¹, GREGORY MALINOWSKI⁴, MICHEL HEHN⁴, MATIAS BARGHER^{2,3}, and ANDERS MADSEN¹ — ¹European XFEL, Germany — ²Institut für Physik und Astronomie, Universität Potsdam, Germany — ³Helmholtz-Zentrum Berlin, Germany — ⁴Institut Jean Lamour, Université Lorraine, France

The transport of heat (or energy in general) in nanoscopic heterostructures is of great interest on a fundamental as well as a technological level, e.g. in the context of thermal management in devices or heat-assisted magnetic recording. In metal heterostructures, heat can be conducted by electrons that are in or out of equilibrium with lattice vibrations. Using ultrafast x-ray diffraction (UXRD), we investigate the influence of thin layers with high electron-phonon coupling on the thermal transport through a 100 nm Cu/Au layer sandwiched by thin Pt and Ni films on picosecond time scales after femtosecond laser excitation. The MID end-station at European XFEL is able to perform these time-resolved laser-pump x-ray-probe measurements to track the time dependence of the heat transport.

A time-dependent diffusive two temperature transport model reproduces our experimental data and thus verifies the efficient transport channel from the laser excited Pt-layer to the Ni-layer via hot electrons.

MM 12.4 Mon 18:15 P2/OG1+2

Structural evolution and atomic transport in severely deformed bi-metallic samples — ●SHRADHA V. SEVLIKAR, GERHARD WILDE, and SERGIY V. DIVINSKIY — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Münster, Germany

Mechanical mixing, deformation-induced transport, and chemically-driven diffusion in layered bi-metallic Ni/Cr, Ni/Cu, Cu/Ag, and Cu/Au systems are investigated using scanning- and transmission electron microscopy, electron probe microanalysis and secondary ion mass spectroscopy. Alternatively, stacked Ni/Cr, Ni/Cu, Cu/Ag, and Cu/Au layers were subjected to room temperature high pressure torsion (HPT) using 10 and more revolutions. Atomic mixing is observed and discussed in terms of a high dislocation density, high concentration of non-equilibrium vacancies, and an impact of grain boundaries. The role of creep deformation is addressed by performing shear compression tests at selected temperatures on specially designed Ni or Cu samples with layers of Cr/Cu or Ag/Au deposited on the gauge sections. Mechanical mixing-induced recrystallization in the Cu-Au and Cu-Ag systems is observed and is discussed.

MM 12.5 Mon 18:15 P2/OG1+2

Study of Electron Transport in a DNA model — ●JORGE CARDENAS-GAMBOA¹, JOSÉ GARCÍA², and SOLMAR VARELA^{1,3} — ¹Yachay Tech University, School of Chemical Sciences & Engineering, 100119-Urcuquí, Ecuador — ²Institu Català de Nanociència i Nanotecnologia (ICN2), 08193-Barcelona, España — ³Institute for Materials Science and Nanotechnology, Technische Universität Dresden, Dresden 01062, Germany

In this work, we use the Landauer-Buttiker formula as implemented in the package KWANT (Python library) for studying quantum transport in a DNA molecule based in an analytical tight-binding Hamiltonian recently developed. In our simulation, we used a Hamiltonian considering a kinetic term, a term for intrinsic Spin-Orbit (SO) interaction related to the atomic SO coupling, and a Rashba interaction due to the electric dipoles associated with hydrogen bonds between the bases of the double strand of DNA and we tested the effect of magnetic and no-magnetic leads in the spin-selectivity of the molecule. We obtained that in our model, the spin-orbit coupling associated with the molecule can not be enough to explain the spin selectivity, however, in a system with presence of ferromagnetic leads, enhance the spin selectivity when it is included, which could explain the selectivity observed in similar experiments.

MM 12.6 Mon 18:15 P2/OG1+2

Investigations on thermal contact conductance between filled polymer composites and solids using micro thermography — ●OLIVER ROSER^{1,2}, ANDREAS GRIESINGER³, and OTHMAR MARTI² — ¹Center for Heat Management (ZFW), Stuttgart — ²Institute of Experimental Physics, Ulm University — ³Baden-Wuerttemberg Cooperative State University (DHBW) Stuttgart

When optimizing cooling paths in electronic devices, thermal interface materials (TIMs) are used to optimize the thermal transfer between two solid surfaces. TIMs are thermally conductive filled polymer composites with a complex microstructure. We investigated the intrinsic thermal conductivity of TIMs and the thermal contact conductance between TIMs and solid substrate surfaces using micro thermography. The physical principles of thermal transport when considering this kind of contact have not yet been investigated in detail and just a few experimental results are available. Most common measurement techniques determine a macroscopic conductance. Random surface and filler structures however, cause several variations and some specific effects on contact conductance, which need to be investigated on a microscale. With the utilized IR camera system, we can take pictures with a resolution of down to 14 microns per pixel. The new method allows us to analyze the microscopic heat paths on the particle scale and to understand the physical principles of heat transport in contact zones of TIMs. The main parameters which affect the contact conductance were identified and will be presented in addition to comparisons to other measurement methods, and a microscale simulation approach.

MM 12.7 Mon 18:15 P2/OG1+2

Hydrogen Diffusion in High-Pressure Torsion (HPT) deformed Magnesium and Magnesium-alloys — ●GIORGIA GUARDI¹, SABINE SCHLABACH^{1,2,3}, JULIA IVANISENKO^{2,3}, STEFAN WAGNER¹, 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 is considered a promising material for solid-state Hydrogen storage due to the high achievable gravimetric density of 7.6 wt.% upon Magnesium Hydride (MgH_2) formation. There are however limitations to its practical application, mainly due to the low diffusion rate of Hydrogen in the Magnesium hydride phase, which leads to slow absorption kinetics. A possible way to improve hydrogen kinetics in Magnesium hydride is by increasing the volume fraction of grain boundaries, which can act as fast-diffusion pathways; this can be achieved in bulk samples by severe plastic deformation. In this work we use High-Pressure Torsion (HPT) to increase the grain boundaries concentration in bulk Mg and Mg-Zn-Zr alloys (ZK30 and ZK60) and we investigate how this affects hydrogen diffusion. The diffusivity of hydrogen in Magnesium is evaluated by gas volumetry at room temperature.

MM 12.8 Mon 18:15 P2/OG1+2

A systematic investigation of metastable phases in Niobium using density-functional theory — ●SUSANNE KUNZMANN¹, GABI SCHIERNING¹, and ANNA GRÜNEBOHM² — ¹Universität Bielefeld, Germany — ²Ruhr-Universität Bochum

Although Niobium is a well studied transition metal, it exhibits anomalies such as type II superconductivity, unusual instabilities under pressure. Furthermore a martensitic phase transition has been reported, which is still under debate and raises questions concerning the source.

The present work attempts to approach these previously unexplained observations in a multifaceted manner. Using density functional theory we investigate low energy metastable phases, their instability against

deformation and potential transition paths to bcc ground state for selected phases and the influence of Tantalum contamination. We find both A15 and Pnma phases to be potential candidates for distorted Niobium, as they are low in energy and we discuss a simple transition path with a low energy barrier for the latter.

MM 12.9 Mon 18:15 P2/OG1+2

Computational local point-based boundary conditions method for eigenfrequencies in microwave eccentric spherical cavities — ●ZOYA EREMENKO¹, IGOR VOLOVICHEV¹, OLEKSIY BRESLAVETS¹, and GRIGORIOS ZOUROS² — ¹O. Ya. Usikov Inst. for Rad. & Electr. Nat. Acad. of Sci. of Ukraine Kharkiv, Ukraine — ²School of Electrical & Comp. Eng. Nat. Tech. Univ. of Athens, Athens, Greece

We have elaborated a new method for solving the electrodynamic problem for a resonant structure like a spherical cavity with a spherical dielectric inhomogeneity is randomly located without any limitations. The main feature of the method is the ability to satisfy the boundary conditions at the interface between two dielectric media at individual points located on these boundaries. There is no need to integrate and formulate boundary conditions for each basic mode, as it is usually done by classical methods for solving electrodynamic problems in the frequency domain. We carry out a numerical study to compute the eigenfrequencies in such eccentric configurations. We validate the results and compare the computational efficiency of our method with HFSS commercial software.

MM 12.10 Mon 18:15 P2/OG1+2

Machine learning force fields in VASP — ●FERENC KARSAI¹, ANDREAS SINGRABER¹, JONATHAN LAHNSTEINER¹, RYOSUKE JINNOUCHI², and GEORG KRESSE² — ¹VASP Software GmbH, Sensengasse 8, Vienna, Austria — ²University of Vienna, Department of Physics, Kolingasse 14-16, Vienna, Austria

An efficient and robust method for on-the-fly machine learning force fields implemented into the Vienna Ab-initio Simulation Package (VASP) is presented. This method realizes the automatic generation of machine learning force fields on the basis of Bayesian inference during molecular-dynamics simulations, where the first-principles calculations are only executed when new configurations out of already sampled data sets appear. The power of the method is demonstrated in several applications such as e.g. melting points of ionic and covalent compounds, thermal transport in Zirconia, delta-learning of Carbon monoxide adsorbed on transition-metal surfaces and solid-solid phase transitions in perovskites. The applications show that during learning 99% of the ab-initio calculations are skipped. The implementation of our on-the-fly learning scheme is fully automatized and is mainly controlled by a few parameters. Hence one can optimally sample through a large phase space and the amount of human intervention for the usually laborious task of training is drastically reduced. Finally, the calculations are accelerated by more than 4 orders of magnitude compared to ab initio, while the accuracy remains the same.

MM 12.11 Mon 18:15 P2/OG1+2

Structure prediction of iron hydrides at high pressures by machine-learned interatomic potentials — ●HOSSEIN TAHMASBI¹, KUSHAL RAMAKRISHNA¹, MANI LOKAMANI¹, MANDY BETHKENHAGEN², and ATTILA CANGI¹ — ¹Center for Advanced Systems Understanding (CASUS), HZDR, Görlitz, Germany — ²CNRS, ENS de Lyon, Laboratoire de Géologie, Lyon, France

The structure and properties of iron hydrides under pressure have been of interest to geoscientists. At ambient conditions, there are no stable solid iron hydrides. Previous theoretical and experimental studies suggest that the double hcp phase of FeH is stable at low pressures with phase transitions to the hcp and fcc phases up to 80 and 140 GPa, respectively. Here, we present a theoretical investigation of the potential energy surfaces of FeH at high pressure. We construct a highly transferable machine-learned interatomic potential with a hierarchical approach using the PyFLAME code. Then, using this fast and accurate neural network potential, we systematically explore the potential energy surfaces of bulk structures of FeH by global sampling using the minima hopping method, to predict stable and metastable iron hydrides up to 200 GPa. We have carried out density functional theory calculations to refine the predicted structures and to evaluate the dynamical stability of selected structures as well. In an automated and systematic approach, we are going to show how a transferable machine-learned interatomic potential can be trained and validated using global optimization and analyze the phase diagram of the stoichiometric Fe-H

system under pressure.

MM 12.12 Mon 18:15 P2/OG1+2

Machine Learning Interatomic Potentials for amorphous mesoporous metallosilicates — ●JULIAN GREIF, KONSTANTIN GUBAEV, and BLAZEJ GRABOWSKI — Universität Stuttgart, D-70049, Stuttgart, Germany

Improving the efficiency of catalysis continues to be an important topic in modern chemistry. A promising approach currently under investigation is to utilize molecular catalysts in confined geometries. In the present project, we aim to model porous amorphous silica containing metal atoms on the pore surfaces that can act as co-catalysts. We conduct atomistic simulations using ab initio-trained machine learning potentials to obtain insights into the location of the metal atoms and the chemical configuration of hydrogen saturated surfaces in the silica structure. To that end, a potential capable of simulating the remelting of $\text{SiO}_2 + \text{Al}$ was trained and checked on the bulk amorphous SiO_2 -system against experimental data in terms of realistic densities, bond lengths and bond angles. Using this potential, new structures are then created by melting and quenching and a new potential is trained for simulations of mesoscale cells.

MM 12.13 Mon 18:15 P2/OG1+2

Deep learning for generation of optimal reaction environments — ●RHYAN BARRETT¹ and JULIA WESTERMAIR² — ¹Leipzig University — ²Leipzig University

The design of reaction environments to reduce activation energies holds enormous potential for advancing many areas of chemical engineering but remains a difficult task due to the high combinatorial complexity of different conditions that influence a reaction. Herein, we use a cutting-edge deep learning model to enable the optimization of reactions. Initially we use a model to generate an abstract electrostatic field that reduces the activation barrier of a given reaction. We then look to optimize the ratio of continuum solvents to match the influence of the optimal electrostatic field generated by the model. The advantage of our method is that it is not limited to the initial solvent selection since any designed mixture will be compared with the global optimum electrostatic field produced by our model. The potential of the method will be demonstrated by optimization of the Claisen rearrangement reaction of allyl-p-tolyl ether and construction of an optimal environment but is generally applicable to any organic reaction.

MM 12.14 Mon 18:15 P2/OG1+2

Efficient graph neural networks for accurate interatomic potentials between surfaces and adsorbed atoms — ●NIAN WU¹, FABIO PRIANTE¹, ERIC KRAMER ROSADO¹, and ADAM S FOSTER^{1,2} — ¹Department of Applied Physics, Aalto University, 00076, Espoo, Finland — ²WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Various advanced microscopy techniques have been developed to resolve molecular systems on surfaces with increasing resolution. However, 2D images representing 3D structures generally lead to missing information, making the interpretation of images challenging. Density functional theory (DFT) with explicit 3D structures offer a route to understanding through analyzing multiple molecular conformations, but the DFT is extremely computationally demanding. To address this issue, in this work we train a neural network potential to predict the interatomic interactions between adsorbates and surfaces as an efficient substitute for DFT calculations with decent accuracy. Firstly, we established a dataset of 2000 organic molecules adsorbed on the Cu(111) surface either in equilibrium or distorted, which includes total energy, atomic force, electrostatic potential, and charge obtained by DFT calculations. And then, based on the small training dataset, we further developed a model on a basis of the NequIP framework, to predict forces. With the auxiliary information from charge and electrostatic potential, our modified model could reach state-of-the-art performance with forces mean absolute errors of ~ 1.0 meV/atom, comparable to DFT accuracy.

MM 12.15 Mon 18:15 P2/OG1+2

Investigation of bonding mechanism between early transition metals and antimony — ●CAROLIN PETERSEN, CHRISTIAN STENZ, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University

Using density functional theory (DFT) one can calculate the number of electron transferred (ET) and electron shared (ES) for crystalline

materials. By plotting ET and ES for different materials on the x- and y- axes, the so-called bonding map is created. It can categorize the different bonding mechanisms, like covalent, ionic, metallic or metavalent and can predict properties such as the band gap, effective coordination number, electrical conductivity, or Born effective charge.

This algorithm works especially for crystalline s- and p-bonded materials. Due to the complexity of d-orbitals in early transition metals, it is unclear how to reasonably normalize ET in that case. The question is where such systems with bonding between d- and p-electrons are located in the bonding map. By examining the properties of such a material, the region in the bonding map can be identified reversely.

Therefore, TiSb is produced by co-sputter deposition and the amorphous phase is investigated by means of electrical transport, e.g. by Hall- and magneto-resistance measurements down to 2K. It is assumed that TiSb is an exotic metal and shows unconventional transport properties.

MM 12.16 Mon 18:15 P2/OG1+2

DFT structural characterization of β - and δ - intermetallic Al-Fe-Si phases — ●NEBAHAT BULUT¹, HANKA BECKER², ANDREAS LEINWEBER², and JENS KORTUS¹ — ¹TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany — ²TU Bergakademie Freiberg, Institute of Materials Science, Germany

The β - $\text{Al}_{4.5}\text{FeSi}$ and δ - Al_3FeSi_2 phases are known stable phases of Fe-containing hypoeutectic Al-Si alloys. Despite the known stoichiometry of the β - and δ - phase the positions of the Al and Si atoms in these Al-Fe-Si intermetallic phases could not be uniquely determined experimentally. Therefore possible positions of Si atoms in these intermetallic phases were investigated using the density functional theory (DFT) code Quantum Espresso, which is based on plane waves and pseudopotentials [2]. For both β - and δ - phase different arrangements of Si atoms in the Al-Fe-Si intermetallics were considered. We compare the energies of these arrangements (1) relaxing the atomic positions keeping the unit cell volume constant and (2) fully relaxing atomic positions and unit cell shape and volume. As result we find that arrangements where the Si atoms are not nearest neighbours are energetically favored [2]. Further, we analyze the electronic structure and investigate the bonding.

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

[2] Becker et al. J. Alloys and Comp. 911 (2022) 165015

MM 12.17 Mon 18:15 P2/OG1+2

A method for charge-sloshing free precise linear-scaling density-functional calculations — ●RUDOLF ZELLER — Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

A fundamental problem for large-scale density-functional calculations is charge sloshing caused by the long-ranged Coulomb potential which necessitates that the number of self-consistency steps increases proportionally to the square of system length. To overcome this problem, Manninen et al. (1975) used a screened Coulomb potential to devise a real-space potential-mixing scheme which in reciprocal space is well-known as Kerker mixing.

It will be described how (1) this scheme works in the linear-scaling real-space code KKRnano which is part of the JuKKR code family developed at the research center Jülich, how (2) it can be turned into a real-space preconditioning method for potential mixing and how (3) it can be refined for excellent numerical performance.

Benchmark calculations will be presented for spin-orbit induced non-collinear magnetism in B20 MnGe and for a vacancy in Cu. It will be shown that the computing effort is drastically reduced, that the number of self-consistency steps does not increase with system size and that precise total-energy differences can be obtained even for supercells with more than 100000 atoms.

It should be noted that the method presented does not rely on using linear response or properties of the static dielectric matrix.

MM 12.18 Mon 18:15 P2/OG1+2

How to Train a Neural Network Potential — ●ALEA MIKAO TOKITA^{1,2} and JÖRG BEHLER^{1,2} — ¹Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany

High-Dimensional Neural Network Potentials (HDNNPs) provide potential energy surfaces (PESSs) with the accuracy of electronic structure calculations at strongly reduced computational costs, which enables extended molecular dynamics simulations of large systems. They are trained on reference energy and force data to learn an approximate but

accurate functional relation between the atomic structure and the PES. However, due to the non-physical functional form, which is shared with many other types of machine learning potentials, this training and the validation of the potential have to be done with great care. In this contribution the construction of HDNNPs will be explained step by step including a discussion of possible pitfalls and tricks of the trade.

MM 12.19 Mon 18:15 P2/OG1+2

PyRamanGUI: An open-source multi-purpose tool to analyze Raman spectra — ●SIMON BREHM, CAMELIU HIMCINSCHI, JAKOB KRAUS, and JENS KORTUS — TU Bergakademie Freiberg, Germany

PyRamanGUI is a software tool which was developed to process and analyze Raman spectra. Available functionalities include smoothing, baseline correction, cosmic spikes removal, peak fitting, and multivariate statistical methods. Furthermore, it is possible to create workflows, which can be personalized and adapted. The application is designed as a graphical user interface (GUI), so no prior knowledge in programming is needed. The program is completely written in python and thus usable across different platforms. The source code is freely available on GitLab (<https://gitlab.com/brehmsi/PyRamanGUI>).

MM 12.20 Mon 18:15 P2/OG1+2

Non-contact friction on various material systems — ●KIM LAMBERT¹, NIKLAS WEBER¹, MATTHIAS KRÜGER², and CYNTHIA VOKERT¹ — ¹Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — ²Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

To gain a deeper understanding of the origins of frictional losses and of how these connect to internal damping in the material, we investigate non-contact friction in various material systems, including graphene flakes and spinodal decomposed systems using AFM-based methods. A main goal of this work is to understand the degrees of freedom that contribute to energy dissipation and to identify the mechanisms contributing to non-contact friction.

For this purpose, we perform friction measurements on these systems under UHV and ambient conditions as well as with different dynamic AFM-based methods. Furthermore, we conduct experiments in contact mode to understand how the damping measured in non-contact is correlated with the energy dissipation measured in contact mode. These insights will be compared to the results of previous studies on [LaMnO₃]_m/[SrMnO₃]_n superlattices [1] as well as to theoretical studies on frictional damping via a theory of viscoelasticity [2].

[1] N. A. Weber et al., arXiv:2210.09677 [2] M. Lee et al., arXiv:2205.01151

MM 12.21 Mon 18:15 P2/OG1+2

Thermodynamical Stability Analysis of a Model Quasicrystal — ●MORITZ HOLZWARH, JOHANNES ROTH, and HANS-RAINER TREBIN — FMQ, Uni Stuttgart, Germany

The random tiling hypothesis, first proposed by Henley in 1991, states that quasicrystals are entropy-stabilized and, hence, are high temperature phases. We confirm the hypothesis for a two-dimensional Tübingen triangle tiling which arises in molecular dynamics simulations with a Lennard-Jones-Gauß potential, by investigating the temperature dependence of its two phason elastic constants λ_6 and λ_8 . These are the second derivatives of the free energy $F(\chi_6, \chi_8, T)$ with respect to the symmetrized phason strain modes χ_6 and χ_8 . At $T = 0$, F has a saddle point by descending along the χ_8 direction. Therefore, $\lambda_8 < 0$ characterizes the quasicrystal's initial instability. The configurational entropy due to phason flips turns F upwards at higher temperatures, reverses the sign of λ_8 and leads to a stable quasicrystal. We obtain this result by applying exclusively geometric methods in the form of the polar calculus, where the atomic domain (AD) is divided into sections for each vertex environment. We extend the calculus to a dynamic one by separating the AD into areas that characterize the different kinds of phason flips. By phasonic deformation of the AD, we can determine the types of flips and their frequency in dependence of phason strain, can perform energy relaxations by flips and compute the configurational entropy. We find that an important mechanism supporting the quasicrystal stability is the symmetric nearest neighbour coupling of phasonic flips.

MM 12.22 Mon 18:15 P2/OG1+2

Excitation-induced non-thermal effects in silicon — ●SIMON KÜMMEL, DOMINIC KLEIN, and JOHANNES ROTH — FMQ University of Stuttgart, Germany

Ultra-fast laser excitation of silicon leads to highly non-linear, non-equilibrium effects in covalent materials. Especially the non-thermal melting in covalent materials like silicon has been observed in experiments. A rigorous explanation in the context of the induced macroscopic material dynamics during laser ablation is still missing. Here, we present novel results from laser ablation simulations taking this effect into account via an electron temperature-dependent interaction potential. We report non-thermal surface evaporation and pre-shockwave melting comparable to experimental investigations. Furthermore, we give more insight into non-thermal melting from electron temperature-dependent phase diagrams obtained from thermodynamic integration of the same electron temperature-dependent interaction potential.

MM 12.23 Mon 18:15 P2/OG1+2

Towards understanding the chemical bonding of unconventional metals — ●CHRISTIAN STENZ, JOHANNES HOLTERS, and MATTHIAS WUTTIG — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany.

Solids can be distinguished based on their properties such as the band gap, effective coordination number, electrical conductivity, Born effective charge and so on. Based on these properties a classification into metallic, covalent, ionic and metavalent bonding seems appropriate. Metavalent bonding is a distinct bonding mechanism characterized by a competition between electron localization and electron delocalization. Chalcogenides like GeTe and Sb₂Te₃ and pnictides like Sb employ this bonding mechanism and can be characterized as 'incipient metals'. This raises the question if there are related metals, which are characterized by the same competition between electron localization and electron delocalization. We thus have been looking for such unconventional metals and focus on compounds of Te with transition metals. The overlap between Te p- and transition metal d- orbitals gives rise to a configuration which resembles the p-p σ -bond in incipient metals. Hence we are looking for related fingerprints such as soft, anharmonic bonds, an unconventional bond rupture and other characteristics which are found for incipient metals.

MM 12.24 Mon 18:15 P2/OG1+2

An efficiently automated method to sample the energies of grain boundaries — ●TIMO SCHMALOFSKI¹, MARTIN KROLL^{2,3}, REBECCA JANISCH¹, and HOLGER DETTE³ — ¹ICAMS, Ruhr-University Bochum — ²Department of Mathematics, Physics, and Computer Science, University of Bayreuth — ³Department of Mathematics, Ruhr-University Bochum

Grain growth and microstructure evolution depend on the anisotropy of the energy of grain boundaries, which is a function of the five geometric degrees of freedom (DOF) of the grain boundaries. To access this parameter space in an efficient way and discover energy cusps in unexplored regions, a method was established, which combines atomistic simulations with statistical methods [1]. It has been successfully applied to sample the 2D subspace of GB plain inclinations for fixed misorientations. The poster explains the main features of the algorithm: Initial design, sequential design, the stopping criterion and the final interpolation of the energy. The algorithm draws its strengths from two aspects, the choice of the next point, which balances a homogeneous distribution of points with a precise sampling of the cusps, and the stopping criterion, which monitors the error of the prediction as well as the number of cusps which have been found. With these features, the method is able to outperform a regular high-throughput sampling.

MM 12.25 Mon 18:15 P2/OG1+2

Cubic scaling GW in the exciting code — ●MANOAR HOSSAIN¹, ALEXANDER BUCCHERI¹, ANDRIS GULANS², and CLAUDIA DRAXL¹ — ¹Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin Germany — ²Department of Physics, University of Latvia, Riga, Latvia

The GW approximation is the state-of-the-art method to incorporate many-body effects through the self-energy correction to the Kohn-Sham single-particle states. A serious drawback is that it becomes often computationally prohibitive due to its typical quartic dependence on system size. This restricts its use to systems with a few tens of atoms, highlighting the need to develop computationally efficient algorithms to extend the computation of the quasi-particle electronic structure to materials consisting of hundreds of atoms. In this work, we present a cubic-scaling algorithm implementation of the GW approximation in the exciting[1] code which is based on the linearized augmented planewave method. Our implementation employs the real-

space imaginary-time formalism[2, 3] and relies heavily on Fast Fourier Transforms and efficient linear-algebra operations. To this extent we develop and make use of high-performance libraries, within the NOMAD CoE[4] with the aim to bring GW to exascale performance.

- [1] A. Gulans, et al. *J. Phys.: Condens. Matter* 26, 363202 (2014).
- [2] P. Liu, et al. *Phys. Rev. B* 94, 165109 (2016).
- [3] A. L. Kutepov, et al. *Comp. Phys. Commun.* 219, 407 (2017).
- [4] <https://nomad-coe.eu>

MM 12.26 Mon 18:15 P2/OG1+2

Physics Informed Neural Networks based Solvers for the Time-Dependent Schrödinger Equation — ●KARAN SHAH and ATTILA CANGI — Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

We demonstrate the utility of Physics Informed Neural Network based solvers for the solution of the Time-Dependent Schrödinger Equation. We study the performance and generalisability of PINN solvers on a simple quantum system. The method developed here can be potentially extended as a surrogate model for Time-Dependent Density Functional Theory, enabling the simulation of large-scale calculations of electron dynamics in matter exposed to strong electromagnetic fields, high temperatures, and pressures.

MM 12.27 Mon 18:15 P2/OG1+2

High-throughput calculations for property maps of solids — ●DANIELA IVANOVA¹, DANIEL WORTMANN¹, STEFAN BLÜGEL¹, MATTHIAS WUTTIG², and CARL-FRIEDRICH SCHÖN² — ¹Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — ²Department of Physics, RWTH Aachen University, Aachen, Germany

Over the last two decades, high-throughput computations have become a vital pillar of the scientific research and development process in the field of computational science. In order to forecast material properties for larger sets of atomic configurations, Density Functional Theory (DFT) has been employed as an automated, robust, and highly-predictive first-principles approach. In this work, the DFT code Quantum ESPRESSO is deployed through the open source Automated Inter-active Infrastructure and Database for Computational Science AiiDA framework. 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 recently been found for another bonding mechanism in solids such as crystalline chalcogenides, termed as (6) 'metavalent bonding'. Effective mass calculations promise essential data for mapping distinctions between the bonding mechanisms along the materials data set chosen for high-throughput computing.

MM 12.28 Mon 18:15 P2/OG1+2

A high-level workflow-based approach towards the exploration of magnetocaloric Heusler alloys by automated high-throughput simulations — ●SIMON BEKEMEIER¹, ALISA CHIRKOVA¹, and CHRISTIAN SCHRÖDER^{1,2} — ¹Bielefeld Institute for Applied Materials Research, FH Bielefeld — ²Faculty of Physics, Bielefeld University

Digitalization poses a huge chance to accelerate knowledge generation and materials discovery. Due to increasing computational capacities ever more materials data and simulations can be processed. Still the underlying processing and simulations often must be run by scientists manually, slowing down the digital process and hindering the usage of its full potential. One major issue is the translation between tools, to concatenate the tools required to transform given input data via several steps into the wanted output. We present one 'workflow' to calculate entropy change induced by the magnetocaloric effect starting from a description of the material under consideration. It consists of several simulation steps using different methods: from DFT, via spin dynamics simulation, to calculating the entropy change. It allows our group to perform high-throughput simulations but also enables exchange of simulational tools with other scientists, who otherwise need to develop and handle those tools themselves. Especially, experimentalists are enabled to use simulations to further enhance their knowledge generation process by extending their work with theoretical simulations on their own. Furthermore such a workflow opens doors to use AI methods to reveal relations, that were unknown before.

MM 12.29 Mon 18:15 P2/OG1+2

Ontology-Template-Based Description of Anisotropic Conductivity Measurements — ●LENNART SCHWAN^{1,2}, MICHAEL

FEIGE², MORITZ BLUHM³, BASIL ELL³, ANDREAS HÜTTEN², and SONJA SCHÖNING¹ — ¹Bielefeld Institute for Applied Materials Research (BIFAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences — ²Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics — ³Semantic Computing Group, Bielefeld University, Faculty of Technology

Digitalization in materials science is an emerging field of research that opens up many new opportunities, e.g. in materials engineering. In particular, if large data sets of many experiments can be evaluated with the help of artificial intelligence. The more information about production, characterization, etc. can be recorded and processed in a machine-readable form, the greater the additional benefit.

A particular challenge is to transfer information that would be recorded in the classic lab book with a simple sketch into a machine-readable form, like the exact position of a measurement. However, this data is important for the evaluation of the experiment.

The application considered is the 3D printing of conductive nanosilver and the determination of the anisotropic electrical conductivity. We semantically describe printing process, environment parameters and characterization in an ontology to investigate dependencies of the conductivity. Therefore, we developed a template-based ontology engineering approach with OTTR templates, to add an abstraction layer to the common but very technical ontology engineering processes.

MM 12.30 Mon 18:15 P2/OG1+2

An Ontology of Magnetocaloric Materials Research — SIMON BEKEMEIER¹, MORITZ BLUM², LUANA CARON³, PHILIPP CIMIANO², BASIL ELL², INGA ENNEN³, MICHAEL FEIGE¹, THOMAS HILBIG¹, ANDREAS HÜTTEN³, GÜNTER REISS³, TAPAS SAMANTA³, SONJA SCHÖNING¹, CHRISTIAN SCHRÖDER^{1,3}, LENNART SCHWAN^{1,3}, and ●MARTIN WORTMANN³ — ¹Bielefeld Institute for Applied Materials Research, University of Applied Sciences Bielefeld, Interaktion 1, 33619 Bielefeld, Germany — ²Faculty of Technology and CITEC, Inspiration 1, 33619 Bielefeld, Germany — ³Faculty of Physics, Bielefeld University, 33501 Bielefeld, Germany

Magnetic refrigeration based on the magnetocaloric effect is an energy-saving and environmentally friendly alternative to compression based cooling. The cooling effect is based on the heat release or uptake during a magnetic phase-transitions of a magnetocaloric material that can be controlled by a magnetic field. The decades-long search for an alloy suitable for mass application could be made much more efficient by digitizing the scientific process chain. The research project DiProMag thus seeks to digitize the entire research procedure from the production and characterization of magnetocaloric materials to their theoretical description and prototypical application. For this purpose, an ontology - that is a structured representation of knowledge - was developed using a hierarchical template-based approach for the acquisition, semantic representation and abstraction of raw ontological data. The focus of the project is on the advancement of Heusler alloys, with Co₂CrAl serving as the first promising model system.

MM 12.31 Mon 18:15 P2/OG1+2

Laser processing of metal materials created by additive technologies. Optimization of structure and mechanical properties — ●IRYNA GALSTIAN¹, EVGEN LEN¹, TOBIAS GUSTMANN², and NICOLE GEISSLER² — ¹G. V. Kurdyumov Institute for Metal Physics of the N.A.S.U. Kyiv, Ukraine — ²IFW Institute for Complex Materials. Dresden, Germany

In this work, the authors investigated the physical regularities of the structural-phase and chemical state formation in the volume of 3D printed titanium products consisting of several layers (surface layers of 3D printed alloys in the original and modified state and transition zones surface layers of 3D printed alloys in the original and modified state and transition zones) depending on the applied methods and regimes of obtaining and high-energy processing. The authors of the method provided a physical justification of the effectiveness of the combination of electron beam 3D printing with surface treatment by means of precision gas dynamic 3D printing and laser treatment. It has been established that this approach makes it possible to eliminate the main disadvantages of 3D-printed alloys, which are their structural imperfection, which causes low plasticity, fatigue strength and corrosion resistance. From a fundamental point of view, it allows to give a complete physical picture of the process of forming the structure and physical and mechanical properties of metal materials during 3D printing and to find ways of managing this process.

MM 12.32 Mon 18:15 P2/OG1+2

MD Simulation of 3D Laser Printing — ●JONAS SCHMID, KEVIN VIETZ, DOMINIC KLEIN, and JOHANNES ROTH — FMQ University of Stuttgart, Stuttgart, Germany

While most people associate the manufacturing of metal parts with a CNC milling machine, the Fraunhofer Society developed an additive manufacturing process in 1995 which is based on laser melting of a metal powder. In this process, metal components are printed layer by layer, while the metal powder is fused onto the previous layer.

Our research focuses on developing molecular dynamics (MD) simulations of 3D laser printing in order to study defects such as gas pockets, cracks or structural irregularities caused by the manufacturing process. In contrast to finite element method calculations, MD simulations describe the highly non-equilibrium dynamics on an atomistic scale. This allows for a more physical interpretation while making less assumptions on the system.

In particular, our simulated system contains a three-dimensional multi-layer powder structure on a fixed ground surrounded by a protective gas. The simulation features laser absorption depending on atom density and atom type, as well as active cooling by using a different thermostat integrator for the ground layer. The overall goal of our research is to optimize the laser and powder properties to reduce defects and increase the stress resistance of the sample.

MM 12.33 Mon 18:15 P2/OG1+2

Molecular dynamics simulation of additive manufacturing: A highly non-equilibrated business — ●KEVIN VIETZ, AZAD GORGIS, DOMINIC KLEIN, and JOHANNES ROTH — FMQ University of Stuttgart, Germany

Powder-bed additive manufacturing is a process that melts the powder with a laser beam, layer upon layer. By performing this melting-solidification process several times, one can build three-dimensional samples. This process is known as 3D printing. Up to now, most simulation studies on additive manufacturing rely on pure metals in vacuum. To fill this gap, we investigate the influence of argon gas on pure metals and explore the suitability of binary alloys for various initial cluster structures, such as core-shell-clusters. We perform large-scale molecular dynamics simulations to depict the highly non-equilibrium material dynamics and evaluate our results by analyzing defects and properties on microscopic and macroscopic scales. Results show that the argon gas stabilizes the system and new material compositions could enhance the variety of applicable materials for additive manufacturing.

MM 12.34 Mon 18:15 P2/OG1+2

Atomistic simulations of crack-tip interface interactions in lamellar TiAl microstructures — ●ONUR CAN SEN and REBECCA JANISCH — ICAMS, Ruhr-University Bochum, Germany

Molecular dynamics simulations are an excellent tool for understanding crack-tip interactions in interface-dominated microstructures, but the simulation setup can affect the predicted behavior as there are many degrees of freedom. To shed light on this and at the same time to understand the impact of the specific interface structure, a systematic study of crack-tip interface interactions in nano-lamellar two-phase TiAl was carried out. To separate microstructure and crack geometry influences, the type of interface, crack configuration, and loading direction were varied in these simulations. Results show that the semi-coherent γ -pseudo twin interface is the strongest barrier for the crack propagation while the coherent true twin interface is the weakest. The analysis of the contributing factors shows, that the crack orientation has more influence on the crack evolution than the crack aspect ratio. The effect of the individual interfaces can be quantified by calculating their shielding effects, but as it turns out this effect is strongly dependent on the crack configuration. However, regardless of the crack configurations, the coherent γ -true twin interface appears to be the most effective interface in terms of shielding.

MM 12.35 Mon 18:15 P2/OG1+2

Overview of Crack-Heterogeneity Interactions at the Atomic Scale — ●LEON PYKA¹, TARAKESHWAR LAKSHMIPATHY², and ERIK

BITZEK² — ¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ²Department Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The study of nano- and microstructure is crucially important for creating materials with more favorable mechanical properties. Specifically in the design of fracture resistant materials, the interaction of cracks with other heterogeneities plays a vital role. In this regard classical atomistic simulations are beneficial. They allow us to gain information on crack-heterogeneity interactions, some of which require sample sizes too large for more accurate electronic structure methods. This information can then be used to improve meso- and continuum-scale models.

We provide an overview of a variety of crack-heterogeneity interactions studied at the atomic scale and their relation to established models. Some simulations of cracks interacting with heterogeneities are also performed using a nearest neighbour "snapping-spring" harmonic potential. In addition to providing material-generic insights, due to the linear interatomic force interactions such potentials allow for direct comparisons with continuum models based on linear elasticity.

MM 12.36 Mon 18:15 P2/OG1+2

Fracture surface energy of glasses obtained from crystalline structure and bond energy data — ●MARCO HOLZER¹, TINA WAURISCHK¹, JANINE GEORGE^{1,2}, ROBERT MAASS^{1,3}, and RALF MÜLLER¹ — ¹Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — ²Institute of Condensed Matter Theory and Solid-State Optics at Friedrich Schiller University, Jena, Germany — ³Department of Materials Science and Engineering at University of Illinois, Urbana-Champaign, USA

Extending our earlier work on nucleation and surface energies [1], we present a simple approach for predicting the fracture surface energy (g) of oxide glasses using readily available crystallographic structure data and diatomic bond energies. The proposed method assumes that (g) of a glass equals the surface fracture energy of the weakest fracture (cleavage) plane of the isochemical crystal. For non-isochemically crystallizing glasses, an average (g) is calculated from the weighed fracture energy data of the constitutional crystal phases according to Conradt [2]. Our predictions yield good agreement with the glass density- and chemical bond energy-based prediction model of Rouxel [3] and with experimentally obtained (g) values known at present. [1] C. Tielemann, S. Reinsch, R. Maass, J. Deubener, R. Müller, J. Non-Cryst. Solids 2022, 14, 100093 [2] R. Conradt, J. Non-Cryst. Solids 2004, 345-346, 16 [3] R., Tanguy, Scripta Materialia 2017, 109-13, 137

MM 12.37 Mon 18:15 P2/OG1+2

An in situ crack detection approach in additive manufacturing based on acoustic emission and machine learning — ●VIKTORIA NIKONOVA¹, DENYS KONONENKO¹, DMITRY CHERNYAVSKY¹, MIKHAIL SELEZNEV², and JEROEN VAN DEN BRINK^{1,3} — ¹Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — ²Institute of Materials Engineering, Technische Universität Bergakademie Freiberg, Gustav-Zeuner-Straße 5, D-09599, Freiberg, Germany — ³Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

Laser Powder Bed Fusion (LPBF) is a state-of-the-art solution for producing metal elements with complex shapes in various industries, from automotive to aerospace. One of the crucial practical drawbacks of LPBF is the presence of structural defects in the printed part, especially cracks. Here we propose an in situ monitoring system of cracks formation during the LPBF process utilizing acoustic emission and machine learning. We demonstrate that the representation of acoustic emission events in the space of principal components (PC) of the spectra yields a robust differentiation of crack events from the noise bursts. The ML classification algorithms achieve high accuracy of ~99 % for the PC-based descriptors. The presented approach advances the method of in situ quality control systems and brings it closer to practical implementations.

MM 13: Invited Talk: Sinclair

Time: Tuesday 9:30–10:00

Location: SCH A 251

Invited Talk

MM 13.1 Tue 9:30 SCH A 251

Exploring the Slow Dynamics of Interfaces and Glasses via Markov State Models — SIAVASH SOLTANI¹, JOERG ROTTLER^{2,3}, and ●CHAD SINCLAIR¹ — ¹Department of Materials Engineering, The University of British Columbia, Vancouver, BC, Canada V6T 1Z4 — ²Department of Physics and Astronomy, The University of British Columbia, Vancouver, BC, Canada V6T 1Z1 — ³Stewart Blusson Quantum Matter Institute, The University of British Columbia, Vancouver, BC, Canada V6T 1Z4

A persistent challenge for molecular simulations is to assess slow processes efficiently from short trajectories. Important examples of slow phenomena in materials are the motion of interfaces in alloy crystals

or the structural relaxation in glass forming liquids. Markov State Models (MSM) are an attractive tool to unveil the slowest processes of a complex atomistic system in a low dimensional space of feature variables. This talk describes the predictions and insights gained from such MSMs constructed using machine learning techniques. For grain boundaries, the model learns a hierarchy of timescales associated with transformations between geometrically distinct motifs. When applied to a binary glass former, our model finds a transition timescale between states that is larger than the conventional structural alpha-relaxation time. In both systems, the MSMs are able to access kinetics at temperatures where brute force calculations become computationally expensive or impossible.

MM 14: Development of Computational Methods: Thermodynamics and Local Chemistry, Electronic Structure

Time: Tuesday 10:15–13:00

Location: SCH A 251

MM 14.1 Tue 10:15 SCH A 251

Performance of pseudopotentials in chemically diverse materials — ●ANDRIS GULANS¹ and STEFAN GOEDECKER² — ¹University of Latvia, Riga, Latvia — ²University of Basel, Switzerland

We present a novel framework for assessing quality of pseudopotentials. It comprises a database of atomization energies and new highly precise norm-conserving pseudopotentials. The database covers more than 700 molecules with 65 elements from six rows of the periodic table. It accounts for chemical diversity by considering every atom in a variety of oxidation states. For each molecule, we provide highly precise scalar-relativistic atomization energies obtained with linearized augmented plane waves obtained using PBE exchange-correlation functionals. The new pseudopotentials reproduce the reference data within the chemical accuracy limit of 1 kcal/mol. They are crucial for assessing other pseudopotentials, as we use them for decomposing the total error in atomization energies into individual atomic contributions. Our calculations reveal that even state-of-the-art pseudopotential families are still not fully compliant with chemical accuracy, and the largest errors arise in molecules with atoms in high oxidation states.

MM 14.2 Tue 10:30 SCH A 251

Pushing to the limits of machine-learning potentials for high-entropy alloys — ●KONSTANTIN GUBAEV, VICTOR ZAVERKIN, PRASHANTH SRINIVASAN, and BLAZEJ GRABOWSKI — University Stuttgart

Chemically complex multicomponent alloys have garnered widespread interest owing to their exceptional properties coming from a sheer inexhaustible compositional space. The complexity poses severe challenges for atomistic modelling and interatomic potential development. Here, we explore the limits of two complementary state-of-the-art machine-learned potentials—the moment tensor potential (MTP) and the Gaussian moment neural network (GM-NN)—in simultaneously describing both the configurational and vibrational degrees of freedom in the prototype Ta-V-Cr-W alloy family. Both models are equally accurate with exceptional performance in comparison to classical potentials. A single potential is able to achieve root-mean-square-errors of 1.37–4.35 meV/atom and 0.023–0.057 eV/Å in 0 K energies and forces, respectively, across all subsystems of the alloy family, and 0.156–0.179 eV/Å in high-temperature molecular dynamics forces for the disordered quaternary. MTPs achieve faster convergence with the training size than the GM-NNs, whereas GM-NNs are faster in execution. Active learning is partially beneficial and has to be complemented with a conventional human-based training set generation.

MM 14.3 Tue 10:45 SCH A 251

Extracting free energies from local composition fluctuations in solids: Theoretical background and atomistic simulations — DANIEL BITTER¹, MARVIN POUL², GUIDO SCHMITZ¹, and ●SEBASTIAN EICH¹ — ¹Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, D-70569 Stuttgart, Germany — ²Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany

While thermodynamic fluctuation theory has been applied to liquids for decades in order to obtain direct thermodynamic information, i.e. Gibbs free energies, from local composition fluctuations, the present work offers an extension for the application in solids. It is demonstrated that composition fluctuations are affected by an additional elastic work term which arises only in solids, thus covering liquids as a special case. The extended fluctuation model is verified through atomistic simulations in an exemplary Cu–Ni embedded-atom system for which Monte Carlo simulations have been carried out in the semi-grand-canonical ensemble at fixed temperature over the entire composition range. Composition fluctuations were monitored in a sub-volume over time and statistically evaluated in terms of the variance, demonstrating perfect agreement with the prediction from the extended model. This method has been developed primarily for the application to experimental atom probe data, where three-dimensional chemical information is available with sub-nanometer accuracy, allowing a direct measurement of local composition fluctuations to extract thermodynamic information.

MM 14.4 Tue 11:00 SCH A 251

Extracting free energies from local composition fluctuations in solids: Application on the atom probe data obtained from TAPSim simulations — ●JIANSU ZHENG¹, MARVIN POUL², and SEBASTIAN EICH¹ — ¹Institute of Materials Science, University of Stuttgart, Heisenbergstr. 3, D-70569 Stuttgart, Germany — ²Max-Planck-Institute für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany

This work proposes a novel methodology to extract direct thermodynamic information, i.e. Gibbs free energies, from local composition fluctuations found in atom probe data based on statistical mechanics. The proof-of-concept is demonstrated with an exemplary simulated Cu–Ni alloy, which has first been equilibrated using Monte Carlo techniques with an embedded-atom potential and subsequently field evaporated by TAPSim[1]. It is shown that the variance of the local composition on the reconstructed data reveals a significant dependence on the size of the chosen (sub-) volume used for the evaluation, but nevertheless the extrapolation to an infinitely large volume unveils a remarkable link to the curvature of the Gibbs free energy. Given the composition range is explored at several points, the Gibbs excess free energy of mixing could be recovered in a CALPHAD-style parametrization. This methodology promises to improve the accuracy of thermodynamic information from direct atom probe measurements.

[1] C. Oberdorfer, S.M. Eich, G. Schmitz. *Ultramicroscopy* 128, (2013), 55.

MM 14.5 Tue 11:15 SCH A 251

A general-purpose framework for kinetic Monte-Carlo simulations — ●ROYA EBRAHIMI VIAND and SEBASTIAN MATERA — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The kinetic Monte Carlo (kMC) method has gained popularity in the last years for the simulation of problems whose dynamics are controlled by rare events. Applications range from atomic-scale models for het-

erogeneous catalysis or charge transport to disease modeling, and a number of specialized codes have been developed for different classes of models. However, specialization is often the bottleneck when trying to extend the codes to a more general setting or to implement new algorithms. We present our first steps towards a flexible general-purpose framework for implementing kMC models to overcome these limitations. This assumes nothing more than that the model can be regarded as a continuous time, discrete state Markov process, which is common among all kMC models. The specific physical model must be provided by the user in terms of update functions for the transition rates of the different possible elementary processes. Besides illustrating the usage on simple and well investigated models, we demonstrate how the tool can be used to implement models with long range interactions, e.g., for the simulation of charge transport in solid materials.

15 min. break

MM 14.6 Tue 11:45 SCH A 251

Pressure-driven tunable properties of the small-gap chalcopyrite topological quantum material ZnGeSb₂: A first-principles study — ●SURASREE SADHUKHAN¹, BANASREE SADHUKHAN², and SUDIPTA KANUNGO¹ — ¹Indian Institute of Technology Goa, 403401 Ponda, India — ²KTH Royal Institute of Technology, Stockholm

Search for new topological quantum materials is the demand to achieve substantial growth topological phase of matter. In this search process, theoretical prediction is crucial besides the obvious experimental verification. The divination of topological properties in already well-known narrow gap semiconductors is flourishing in quantum material science. We revisited the semiconductor compound in the chalcopyrite series, some of which were potential topological materials. Using this density functional theory-based first-principles calculations, we report a strong topologically nontrivial phase in chalcopyrite ZnGeSb₂, which can act as a model system of strained HgTe. The estimates reveal the non-zero topological invariant (Z_2), Dirac cone crossing in the surface spectral functions with spin-momentum locked spin texture. We also report the tunable topological properties from nontrivial to trivial phases under moderate hydrostatic pressure within *7 GPa. A minor modification of a lattice parameter is enough to achieve this topological phase transition easily accomplished in an experimental lab. We have incorporated the discontinuity in the tetragonal distortion of non-centrosymmetric ZnGeSb₂ to drive the topological quantum phase transition.

MM 14.7 Tue 12:00 SCH A 251

electronic structure of a non-symmorphic kondo lattice system CeAgSb₂ — ●SAWANI DATTA¹, KHADIZA ALI², RAHUL VERMA¹, SAROJ P. DASH², BAHADUR SINGH¹, ARUMUGAM THAMIZHAVEL¹, and KALOBARAN MAITI¹ — ¹Tata institute of fundamental research, Mumbai, India — ²Chalmers university of technology, Goteborg, Sweden

Topological Dirac semimetal with non-symmorphic symmetry (NSS) is one of the most recent discoveries in the field of novel topological quantum materials [1]. The uniqueness of this system is the presence of robust (including spin-orbit coupling) Dirac line nodes with NSS protection. CeAgSb₂, a Kondo system, exhibits a large anisotropic resistivity and a complex magnetic ground state at a lower temperature [2]. Employing angle-resolved photoemission spectroscopy (ARPES), we find that CeAgSb₂ possesses several non-trivial crossings near the Fermi level protected by the NSS. The ARPES data collected at different photon energies suggest a quasi-2-D behavior which is consistent with the transport results. In addition, we observe energy bands of the surface states in the near-Fermi-level region along with the non-trivial bulk bands that make the electronic structure complex. Our study shows the CeAgSb₂ family of materials as a new platform to study the robust non-symmorphic symmetry-protected Dirac semi-metallic systems with high spin-orbit coupling.

[1] L. M. Schoop et. al., Nat. Commun. 7, 11696 (2016). [2] Y. Inada et. al., Philos. Mag. B, 82, 1867 (2002).

MM 14.8 Tue 12:15 SCH A 251

An amplitude expansion of magnetic phase field crystal: A continuum model for magnetically driven dislocation networks — ●RAINER BACKOFEN, MARCO SALVALAGLIO, and AXEL VOIGT — Institute of Scientific Computing, TU Dresden

The amplitude expansion of the phase-field-crystal (APFC) model enables a convenient coarse-grained description of crystalline structures. It allows the description of length scales that are orders of magnitude larger than the lattice spacing while retaining microscopic features, such as dislocations. Adaptive finite elements are used to treat the different involved length scales efficiently [1].

Here, an APFC model is presented that captures the basic physics of magneto-structural interactions: magnetostriction and magnetic anisotropy. The free energy of APFC is combined with a continuum field representing local magnetization [2]. The proposed coupling does not increase the partial differential equation to solve compared with the basic APFC model. Still, it is flexible enough to adapt the magnetic anisotropy of the model to basic ferromagnetic materials such as Fe and Ni. Exploiting this model, the influence of external magnetic fields on the evolution of defects and grain boundaries is discussed.

[1] Salvalaglio, Backofen, Voigt (2018) PRMat, 2(5), 053804. [2] Backofen, Salvalaglio, Voigt (2022) Model Simul Mat Sci Eng

MM 14.9 Tue 12:30 SCH A 251

Multi-orbital models within the ghost Gutzwiller approximation — ●CARLOS MEJUTO-ZAERA and MICHELE FABRIZIO — SISSA, Trieste, Italy

In the pursuit towards targeted material design leveraging strong electronic correlation, computationally inexpensive yet qualitatively reliable methods play a fundamental role. These approaches should allow for a rapid mapping of phase space, unveiling a first impression of possible phases of matter, which can then be explored in selected regions of parameter space with more accurate yet involved techniques. Recently, the ghost Gutzwiller Approximation (gGA) has been shown to be an interesting candidate for this kind of phenomenological search. Based on a self-consistency condition for the simple one-body reduced density matrix of a discretized impurity model, this method can capture spectral features of both coherent and incoherent nature in the one-body Green's function. In this work we extend its applicability to the multi-orbital regime employing a truncated solver based on selected configuration interaction. This allows for increasing the number of correlated orbitals while keeping the size ratio of bath to impurity constant. We explore the reliability of the gGA for describing the phase diagram of multi-band models, comparing to more sophisticated embedding methods. We shall assess the potential of gGA for modelling of complex materials, possibly in combination with ab-initio methods.

MM 14.10 Tue 12:45 SCH A 251

Understanding the success of mGGAs for band gaps. Is it the orbital dependence? — ●PÉTER KOVÁCS, PETER BLAHA, and GEORG K. H. MADSEN — Institute of Materials Chemistry, Technical University of Vienna

Density functional theory has shown remarkable success in predicting various properties of solids, such as lattice parameters and cohesive energies, yet with most functionals it is known to heavily underestimate band gaps. mGGA functionals tend to result in better band gap predictions than LDA or GGAs, but the best results are still achieved at the cost of accuracy for the other properties. Recently using a systematic search in the space of mGGA functionals we were able to find functionals, where this tradeoff is small.[Péter Kovács et al., J. Chem. Phys. 157, 094110 (2022)]

While the failure of LDA and GGA functionals for gaps are often attributed to their lack of the derivative discontinuity, the success of mGGAs can not be explained solely based on their ability to exhibit discontinuous behaviour. On a database of 440 solids, we analyze how two specialized functionals, TASK and our own mGGA23, are able to better predict gaps. We aim to understand what parts of the functional shape is responsible for their success and how these affect their prediction of structural properties, such as lattice parameter. These findings can be used in functional design and also to understand failure cases of already existing functionals.

MM 15: Topical Session: Fundamentals of Fracture – Atomistic Studies of Fracture

Time: Tuesday 10:15–13:00

Location: SCH A 216

Topical Talk MM 15.1 Tue 10:15 SCH A 216
Multiscale Quantum-Atomistic and Atomistic-Continuum Modelling of Crack Propagation — ●JAMES KERMODE — Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, United Kingdom

I will review recent progress on the development and application of advanced algorithms to simulate chemomechanical systems where local chemistry and long-range stress are tightly coupled, e.g. at the tip of a propagating crack or the core of a dislocation. I will discuss two general approaches (i): hybrid quantum/classical approaches where bond-breaking is treated at the DFT level embedded within a large-scale classical atomistic model to capture elastic relaxation, including recent applications to tungsten [1] and diamond [2]; (ii) atomistic-to-continuum modelling for crack propagation, either through extracting effective continuum models from large-scale atomistic simulations of fracture [3], or by flexibly embedding an atomistic domain within a continuum model, using a new algorithm to compute bifurcation diagrams for fracture systems [4].

[1] P. Grigorev et al., arXiv:2111.11262 (2022); [2] J. Brixey, T. Cowie, A. Jardine and J. R. Kermode, In Prep (2022); [3] S. M. Khosrownejad, J. R. Kermode, and L. Pastewka, Phys. Rev. Materials 5, 023602 (2021); [4] M. Buze and J. R. Kermode, Phys. Rev. E 103, 033002 (2021)

MM 15.2 Tue 10:45 SCH A 216
Modelling Fracture in α -Iron via a Numerical-Continuation Scheme — ●LAKSHMI SHENOY¹, ALBERT BARTOK-PARTAY², and JAMES KERMODE¹ — ¹Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry CV4 7AL, United Kingdom — ²Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

I will present results for the stability range of fracture in α -iron mapped using the numerical-continuation flexible boundary scheme (NCFlex) proposed by Buze et. al. [1]. The predictions by two new machine learning interatomic potentials for α -iron [2] - Gaussian approximation potential and atomic cluster expansion - will be compared with those by the classical embedded atom model [3]. From the bifurcation plots produced by NCFlex, the 0K energy barriers to brittle fracture propagation along different crystallographic planes in α -iron will be computed. Using these, a model for the temperature dependence of the brittle-to-ductile transition temperature of α -iron will be proposed, and validated against experimental results. Methods for extending this scheme to finite temperature energy barriers and interaction of the crack tip with point defects will also be discussed.

[1] M. Buze and J. R. Kermode, Phys. Rev. E 103, 033002 (2021) ; [2] Zhang, Lei, et al. arXiv:2208.05912 (2022) ; [3] Mendelev, M. I., et al. Phil. Mag. 83.35 (2003)

MM 15.3 Tue 11:00 SCH A 216
Revealing Atomistic Fracture in BCC Iron by Active Learning — LEI ZHANG¹, GABOR CSANYI², ERIK VAN DER GIESSEN¹, and ●FRANCESCO MARESCA¹ — ¹University of Groningen, Netherlands — ²University of Cambridge, UK

Fracture is multi-scale process that originates from atomic-scale bond rupture and dislocation activity. A clear understanding of these processes is often lacking, because classical interatomic potentials (IAPs) for Molecular Dynamics simulations yield contradicting results that agree only partially with experiments. This is also due to the limited flexibility of their functional form, which is inadequate to describe the complex potential energy surface associated with fracture processes. Emerging machine learning (ML) IAPs allow near-quantum accuracy, based on density functional theory (DFT), but are orders of magnitude faster than DFT. In this work, we develop an active learning algorithm that enables the prediction of atomistic fracture mechanisms via the Gaussian Approximation Potential (GAP) approach. An existing DFT database for ferromagnetic bcc iron is first enriched with configurations that are relevant for the fracture process. Next, the active learning approach is applied to four crack systems, in which the maximum predicted per-atom error is reduced to 10 meV. The predicted critical stress intensity factors are compared with theory estimates, and the learning efficiency of the approach is analysed. Our work provides an active learning strategy for improving ML-IAPs for fracture, while

revealing for the first time the atomic scale mechanisms that initiate fracture in iron with quantum accuracy.

MM 15.4 Tue 11:15 SCH A 216
Benchmarking of Tungsten Potentials using Blunted Cracks — ●TARAKESHWAR LAKSHMIPATHY and ERIK BITZEK — Department Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH

Blunted cracks can have radically different fracture behavior compared to their atomically sharp counterparts due to the additional degrees of freedom available to atoms at the crack tip surface. Simulating realistic notch or crack tip radii requires computationally inexpensive atomic interaction potentials. However, empirical potentials are known to show artefacts like the formation of planar faults at the crack tip due to unrealistic minima in their generalized stacking fault energies or fail to reproduce surface reconstructions. Such drawbacks could play an even larger role in blunted crack simulations than in typically studied sharp cracks due to additional surfaces at the crack tip. In this work, the fracture behavior and fracture toughness of some commonly used EAM potentials are benchmarked against density functional theory (DFT) simulations of blunted cracks in tungsten and compared to recently developed modified-EAM (MEAM), atomic cluster expansion (ACE) and bond order potentials (BOP).

15 min. break

MM 15.5 Tue 11:45 SCH A 216
Development of machine learning interatomic potentials for far-from-equilibrium states: a case study of deformation mechanisms in ceramics — ●SHUYAO LIN¹, DAVIDE SANGIOVANNI², LARS HULTMAN², and NIKOLA KOUTNA¹ — ¹Technical University of Vienna, Institute of Materials Science and Technology, A-1060, Vienna, Austria — ²Linköping University, Department of Physics, SE-58183, Linköping, Sweden

Besides the high chemical stability, the applications of ceramic-based materials into the coating technology require not only high strength but also ductility, a combination of properties necessary for material's resistance to crack growth. The mechanical properties of ceramic materials are dominated by both their movement and interactions. In this talk, we study mechanical response of selected ceramics, including transition metal diborides and nitrides. First, ab initio molecular dynamics simulations (AIMD) are employed to model tensile deformation along main crystallographic directions and under extreme high temperatures with fluid status. Then we develop machine learning interatomic potentials within the moment tensor potential (MTP) framework. The potentials are thoroughly tested and validated against AIMD stress-strain curves. With the aid of newly developed potentials, we carry out large-scale simulations during which the ceramics are continuously loaded and can shrink due to Poisson contractions. The observed deformation mechanisms are described and compared to those present in the small-scale training data.

MM 15.6 Tue 12:00 SCH A 216
Atomistic studies of crack tip twin-boundary interactions in lamellar TiAl alloys: Effect of misfit, misorientation and lamella spacing — ANUPAM NEOGI^{1,2} and ●REBECCA JANISCH¹ — ¹ICAMS, Ruhr-University Bochum, Germany — ²ANSYS Inc., Pune, India

Nano-scale coherent twin boundaries can be an effective way in overcoming the strength-ductility trade-off of metals and their alloys. In this sense also twin boundaries in nano-lamellar lightweight Ti-Al alloys promise a great potential. Furthermore, the existence of three types of these twin boundaries with different misorientation and coherency state at the interface provide an excellent opportunity to study the effect of exactly these parameters in a realistic model system. To this end, we carried out molecular statics simulations to characterize the crack advancement at and across internal true-twins (TTs), rotational boundaries (RBs), and pseudo-twins (PTs) in lamellar γ -TiAl alloys, as well as crack propagation in fully lamellar structures.

It was confirmed that both interface type and spacing affect the fracture toughness and crack growth resistance. Furthermore, the crack tip mechanisms exhibit prominent sensitivity to the crack system and crys-

tallographic directions. For trans-lamellar cracks the tip shows plastic deformation and toughening at all interfaces. The overall fracture initiation toughness in a microstructure of TTs exhibits an increasing trend with decreasing lamellar size down to a critical thickness, below which the fracture toughness drops again. These and more phenomena and their origins will be discussed in the presentation.

MM 15.7 Tue 12:15 SCH A 216

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

The fracture toughness of Tungsten at low temperature is critically influenced by its microstructure. Understanding the underlying crack-microstructure interactions is therefore necessary to model and predict failure. In order to gain insight into the interactions of dislocations with the crack-tip, large scale atomistic simulations are carried out. Dislocations of different character and Burgers vector are placed in the vicinity of a strain controlled crack geometry, resulting either in an attraction or repulsion of the dislocation. In the former case interactions can be observed in the course of the simulation, e.g. cross-slipping of screw parts, changes in crack front or crack plane as well as subsequent dislocation emission. Dependencies on the stress state, the crack system, dislocation type and distance between dislocation and the crack are investigated. The results are discussed with respect to mesoscale and continuum models for crack tip plasticity and fracture toughness.

MM 15.8 Tue 12:30 SCH A 216

Atomistic study of fracture in Laves phases — ●ALIREZA GHAFAROLLAHI and ERIK BITZEK — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf 40237, Germany

Laves phases are intermetallic phases with complex structures that exist in many alloys and have a pronounced impact on their mechanical properties. Although these materials often exhibit superior mechanical

properties at high temperatures, their applications as structural materials are limited due to their intrinsic brittleness at ambient temperature. Therefore, understanding the fundamental fracture mechanisms in Laves phases is crucial for tailoring their mechanical properties. Here, with the aid of atomistic simulations, the fracture behavior in C14 and C15 Laves phases is explored using NbCr₂ and MgZn₂ as model systems. In particular, different crack systems are analyzed and the corresponding fracture toughnesses are computed and compared with the Griffith theory.

MM 15.9 Tue 12:45 SCH A 216

Tailoring negative pressure by crystal defects: Crack induced hydride formation in Al alloys — ●ALI TEHRANCI¹, POULAMI CHARABORTY¹, MARTI LOPEZ FREIXES¹, EUNAN MCENIRY¹, BAPTISTE GAULT^{1,2}, TILMANN HICKEL^{1,3}, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — ²Department of Materials, Imperial College, South Kensington, London, SW7 2AZ, UK — ³Bundesanstalt für Materialforschung und -prüfung (BAM)

Climate change motivates the search for non-carbon-emitting energy generation and storage solutions. Metal hydrides show promising characteristics for this purpose. To enhance the formation and stability of such often highly volatile hydrides we have considered a novel concept: tailoring and employing the negative pressure of microstructural and structural defects to enhance H solubility and thus hydride formation. Using systematic ab initio and atomistic simulations, we demonstrate that an enhancement in the formation of hydrides at the negatively pressurized crack tip region is feasible by increasing the mechanical tensile load on the specimen. The theoretical predictions have been used to reassess and interpret atom probe tomography experiments for a high-strength 7XXX-aluminium alloy that show a substantial enhancement of hydrogen concentration at structural defects near a stress-corrosion crack tip. Based on these insights we derive strategies for enhancing the capability of metals as H-storage materials.

MM 16: Energy Conversion

Time: Tuesday 10:15–13:00

Location: SCH A 215

MM 16.1 Tue 10:15 SCH A 215

Spins at Work: Probing Charging and Discharging of Organic Radical Batteries by Electron Paramagnetic Resonance Spectroscopy — ●ILIA KULIKOV¹, NAITIK PANJWANI¹, ANATOLY VERESHCHAGIN², DOMENIK SPALLEK¹, DANIL LUKIANOV², ELENA ALEXEEVA², OLEG LEVIN¹, and JAN BEHREND¹ — ¹Berlin Joint EPR Lab, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin — ²St. Petersburg, 190034, Russian Federation

We report on the development of an operando setup for spectroelectrochemical Electron Paramagnetic Resonance (EPR) measurements on redox conductive polymers for organic radical batteries. [1]

Quantitative EPR experiments performed on electrochemical cells with a TEMPO containing polymer cathode demonstrate a strong decrease in the number of paramagnetic centres upon oxidation. [2] The distinct EPR signatures of the polymer are used to study its degradation upon repeated cycling. A comparison between the EPR and electrochemical data is used to monitor the degradation process.

Low-temperature ex-situ pulse EPR measurements on an oxidized cathode film reveal a spectrum of dilute nitroxide species, which indicates formation of electrochemically inactive islands. These experiments pave the way for studying organic radical battery materials by advanced EPR techniques.

[1] I. Kulikov et al., Energy and Environmental Science, 2022, 15, 3275.

[2] A. A. Vereshchagin et al., Batteries & Supercaps 2021, 4, 336.

MM 16.2 Tue 10:30 SCH A 215

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 SCHEURER^{1,2} — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²IEK-9, FZ Jülich, Germany

The market quest for fast-charging, long-lasting, safe batteries drives the exploration of new energy storage materials, but also promotes

fundamental studies of those already widely used—primarily graphite anodes for Li-ion batteries. We focus on the upper intercalation limit in the morphologically quasi-ideal highly oriented pyrolytic graphite, with a LiC₆ stoichiometry corresponding to 100% state of charge. A sample prepared by immersion in liquid Li at ambient pressure, investigated by ⁷Li nuclear magnetic resonance (NMR), shows unexpected signatures of superdense intercalation compounds, LiC_{6-x}. These were ruled out for decades, as the highest geometrically accessible composition, LiC₂, can only be prepared under high pressure. We monitored the sample upon calendaric aging and employed DFT calculations to rationalise NMR findings. Computed free energies reveal that non-negligible over-intercalation proceeds spontaneously beyond the currently accepted capacity limit. Challenging the widespread notion that any additional intercalation beyond LiC₆ is not possible under ambient conditions, we highlight the implications on performance-critical phenomena and critically discuss possible quantitative characterization routes[1].

[1] C. Grosu *et al.*, arXiv:2107.11137 (2021)

MM 16.3 Tue 10:45 SCH A 215

Computational investigation of carbon based anode materials for Li- and post-Li ion batteries — ●JAFAR AZIZI¹, HOLGER EUCHNER², and AXEL GROSS¹ — ¹Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany — ²Institute of Physical and Theoretical Chemistry, University of Tübingen, 1572076 Tübingen, Germany

With respect to sodium ion batteries, traditional graphite anodes exhibit a severe limitation due to their inability to intercalate sodium atoms. Hard carbon materials, on the other hand, provide a promising alternative for Na-ion and K-ion batteries with high theoretical capacities and low reaction potentials. The presence of the particular nanostructure of these functionalized carbon-based materials have been shown to be responsible for these features. The major obstacle for a continued development and improvement is a lack of a functional understanding of the role of these structural features with regard to the intercalation and storage mechanism. To overcome these problems, the intercalation of Li, Na, and K in the presence of distinct defects

have been investigated by density functional theory (DFT) calculations. It will be shown how the combination of phonon simulations with electronic band structure calculations allows for a validation of the so-called modified card house model for the alkali metal storage in hard carbon.

MM 16.4 Tue 11:00 SCH A 215

Detailed structural and electrochemical comparison between high potential layered P2-NaMnNi- and doped P2-NaMnNiMg-oxides — ●MANUEL DILLENZ¹, CORNELIUS GAUCKLER², MOHSEN SOTOUDEH¹, HOLGER EUCHNER³, MARIO MARINARO², and AXEL GROSS^{1,4} — ¹Institute of Theoretical Chemistry, Ulm University, Mez-Starck-Haus, Oberberghof 7, 89081 Ulm — ²ZSW-Zentrum für Sonnenenergie und Wasserstoff-Forschung, Helmholtzstrasse 8, 89081, Ulm, Germany — ³Institute of Physical and Theoretical Chemistry, Universität Tübingen, Auf der Morgenstelle 15, 72076 Tübingen, Germany — ⁴Helmholtz Institute Ulm (HIU) for Electrochemical Energy Storage, Helmholtzstraße 11, 89069 Ulm, Germany

Manganese-based transition metal oxides with a P2 structure are promising cathode materials for sodium ion batteries. Although these materials exhibit high working potential vs Na⁺/Na and high capacity, they are affected by Na⁺ ion/vacancy ordering transitions and phase transformations at high voltages, resulting in poor reversibility. Here we present a combined experimental/theoretical approach to investigate the effect of magnesium doping on the layered P2-Na_{0.67}Mn_{0.75}Ni_{0.25}O₂ cathode material. The Mg-doped material showed stabilization of the high potential plateau and improved cycle life. Based on our experimental data and periodic density functional theory (DFT) calculations, phase stabilities of the O2, P2, and OP4 phases for the pristine and Mg-doped systems were investigated to elucidate the origin of the "Z"-phase formation in the Mg-doped systems.

MM 16.5 Tue 11:15 SCH A 215

Coarse-Grained Simulation of Dendrite Growth in Lithium Metal Batteries — ●LEN KIMMS, DIDDO DIDDENS, and ANDREAS HEUER — Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster

In this talk, we will present a simulation study that investigates the formation and growth of dendrites. Due to the increasing demand for portable high-capacity energy storage, there is a renewed interest in Lithium metal batteries (LMBs). In LMBs one electrode is replaced by lithium metal anchored on a current collector. Lithium metal is electrochemically plated on the anode side when charging the battery. Depositing the metal uniformly is a hugely challenging undertaking. The intrinsically high reactivity of lithium metal, electric field effects, and spatial variations of the local composition in the electrolyte all drive dendritic deposition. We employ a versatile coarse-grained model to understand the influence of various electrochemical conditions on the dendrite morphology. The model allows not only the investigation of fundamental driving forces like the electric field and the cation concentration but also the evaluation of more intricate procedures e.g. pulse charging. Different particle types with varying reactivity are implemented, which allows the representation of local passivation. Also, a solid electrolyte interface (SEI) layer can be incorporated either explicitly with a particle layer on the surface or implicitly by modifying the cationic diffusion locally. Here we report results on how to suppress non-uniform deposition by employing charging, microstructured electrode surfaces, and SEI effects.

15 min. break

MM 16.6 Tue 11:45 SCH A 215

Modelling Hard Carbon with High-Dimensional Neural Network Potentials — ●ALEXANDER L. M. KNOLL^{1,2}, JAFAR AZIZ³, HOLGER EUCHNER⁴, AXEL GROSS³, and JÖRG BEHLER^{1,2} — ¹Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany — ³Institut für Theoretische Chemie, Universität Ulm, 89081 Ulm, Germany — ⁴Institut für Physikalische und Theoretische Chemie, Eberhard Karls Universität Tübingen, 72076 Tübingen, Germany

Hard carbon (HC) is widely regarded as a promising anode material for lithium and sodium ion batteries. However, this material is notoriously difficult to characterise experimentally, as its properties strongly depend on the carbon precursor and the conditions of preparation.

Ab initio investigations could help to illuminate its structure, but are severely hampered by its complexity involving large graphitic domains as well as amorphous motifs. To bypass these challenges, we present a high-dimensional neural network potential (HDNNP) for HC that accurately reproduces short-range and dispersion interactions in the system. We show that elaborate structural models can be constructed with this potential using various simulation protocols and demonstrate their validity through comparison to experimental data.

MM 16.7 Tue 12:00 SCH A 215

Computational Studies on the Electrochemical Performance of Doped and Substituted Ti₃C₂T_x (T = O, OH) MXene — ●MANDIRA DAS¹ and SUBHRADIP GHOSH² — ¹Indian Institute of Technology Guwahati, Guwahati, Assam, India — ²Indian Institute of Technology Guwahati, Guwahati, Assam, India

Using Density functional theory (DFT) in conjunction with a solvation model, we have investigated the phenomenon of electrode-electrolyte interaction at the electrode surface and its consequences on the electrochemical properties like the charge storage and total capacitance of doped and substituted functionalized Ti₃C₂T_x (T = O, OH) supercapacitor electrode. We have studied nitrogen-doped, nitrogen substituted, and molybdenum substituted MXenes in acidic electrolyte H₂SO₄ solution. By considering nitrogen doping at different sites, we found that the greatest capacitance is obtained for doping at functional sites. Our results agree well with the available experiment. We also found that the enhancement in capacitances due to nitrogen doping is due to amplifications in the pseudocapacitance. We propose that the primary mechanism leading to the enhanced value of the capacitances due to nitrogen doping is surface redox activity. The performances of substituted systems, on the other hand, are degraded compared to the pristine ones. This suggests that better storage capacities in Ti₃C₂T_x electrode can be obtained by doping only. We provide insights into the reasons behind contrasting behavior in doped and substituted systems and suggest ways to further improve the capacitances in the doped system.

MM 16.8 Tue 12:15 SCH A 215

Structure-property relationships in functionalized metal organic framework from first-principles high-throughput screening — ●JOSHUA EDZARDS¹, HOLGER-DIETRICH SASSNICK¹ 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 (MOFs) are novel materials with high potential in many fields of application, ranging from gas storage and catalysis to optoelectronics. MOFs are constituted by metal atoms bound together by linker molecules which can be modified by functional groups. This leads to an enormous variety of MOFs with different structural properties, which can in turn affect their band structures, projected density of states, charge density distribution, etc. In this project, we perform high-throughput first-principles calculations on MOF-5 a well-known member of the MOF family. We scan all possible structures that arise by exchanging the metal ion Zn with alkaline-earth metals, and by functionalizing the linker molecule (1,4-benzodicycarboxylate) with Br, CH₃, Cl, COOH, NO₂, and OH. We investigate the electronic properties of the stable structures and assess how they are influenced by the choice of the metal ion and by the functionalization of the linkers.

MM 16.9 Tue 12:30 SCH A 215

Lithium diffusion visualized in Li₄+xTi₅O₁₂ using optical microscopy (revealing slow-moving phase boundary) — ●YUG JOSHI, ROBERT LAWITZKI, and GUIDO SCHMITZ — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Stuttgart, Germany

Lithium titanate (Li₄Ti₅O₁₂) undergoes a phase transformation from spinel structured (Li₄Ti₅O₁₂) to rock-salt (Li₇Ti₅O₁₂). The material has been reported to show sluggish mobility of lithium in fully lithiated and delithiated phases. This challenges the high-rate performance observed in this material. To elucidate this behavior, optical microscopy and the electrochromic character of the material have been used to visualize the phase transformation. The kinetics of lithium transport is observed in a constrained region of sputter-deposited thin-film samples. This enables a study of the lateral transport on the length scales of tens of micrometers. Furthermore, with a thermostatically controlled cell, the Arrhenius-like temperature dependence of lithium diffusivity is revealed. Our quantitative findings demonstrate that indeed the end phases have poor diffusivity. Surprisingly, the phase boundary moves

slowly upon lithiation, which has been refuted in prior reports, however, it is confirmed here by the linear growth kinetics of the Li-rich phase in the initial stages of the lithium transport. Interestingly, the partial solubility of lithium in the spinel structured $\text{Li}_4/3+\delta\text{Ti}_5/3\text{O}_4$ phase increases the diffusivity of lithium drastically. This increase in diffusivity along with the reduction in size of the electrode seems to be compensating the kinetic hindrance induced by the phase boundary.

MM 16.10 Tue 12:45 SCH A 215

Photocatalytic water splitting from Koopmans spectral functionals: The case of TiO_2 polymorphs — ●MARIJA STOJKOVIC¹, EDWARD LINSKOTT¹, and NICOLA MARZARI^{1,2} — ¹Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École

Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — ²Laboratory for Materials Simulations, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Photocatalytic water splitting has drawn considerable attention for renewable energy production. Since the first reported photocatalytic water splitting by titanium dioxide, this material remains one of the most promising photocatalysts, due to its suitable band gap and band-edge positions. However, estimating both of these properties is a challenging task for standard DFT functionals. Here we show how Koopmans spectral functionals can accurately predict the band structure and level alignment of rutile, anatase and brookite, demonstrating the advantage of orbital-density dependent functionals for predicting the spectral properties of materials.

MM 17: Phase Transformations: Microstructural Transformations

Time: Tuesday 10:15–11:15

Location: SCH A 118

MM 17.1 Tue 10:15 SCH A 118

About the transformation speed of martensitic transformations — ●SEBASTIAN FÄHLER¹, STEFAN SCHWABE², KLARA LÜNSER¹, DANIEL SCHMIDT³, KORNELIUS NIELSCH³, and PETER GAAL³ — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Leibniz IFW Dresden, Dresden, Germany — ³Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

Structural martensitic transformations enable various applications, which range from high stroke actuation and sensing to energy efficient magnetocaloric refrigeration and thermomagnetic energy harvesting. All these emerging applications benefit from a fast transformation, but up to now the speed limit of martensitic transformations has not been explored. Here, we demonstrate that a martensite to austenite transformation can be completed in under ten nanoseconds. We heat an epitaxial Ni-Mn-Ga film with a laser pulse and use synchrotron diffraction to probe the influence of initial sample temperature and overheating on transformation rate and ratio. We demonstrate that an increase of thermal energy drives this transformation faster. Though the observed speed limit of $2.5 \times 10^{27} \text{ (Js)}^{-1}$ per unit cell leaves plenty of room for a further acceleration of applications, our analysis reveals that the practical limit will be the energy required for switching. Our experiments unveil that martensitic transformations obey similar speed limits as in microelectronics, which are expressed by the Margolus-Levitin theorem.

[1] S. Schwabe, K. Lünser, D. Schmidt, K. Nielsch, P. Gaal and S. Fähler, *Science and Technology of Advanced Materials*, 23 (2022) 633

MM 17.2 Tue 10:30 SCH A 118

Solving the 3D puzzle of the martensitic microstructure in epitaxial NiTi films — ●KLARA LÜNSER^{1,2,3}, ANDREAS UNDISZ^{4,5}, KORNELIUS NIELSCH^{2,3}, and SEBASTIAN FÄHLER¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Leibniz IFW Dresden, Dresden, Germany — ³TU Dresden, Dresden, Germany — ⁴TU Chemnitz, Chemnitz, Germany — ⁵Friedrich-Schiller-Universität Jena, Jena, Germany

The shape memory effect in the most frequently used shape memory alloy NiTi is driven by a martensitic transformation, resulting in a complex martensitic microstructure with a variety of interfaces. As shape memory properties depend on the microstructure, a detailed understanding is crucial. However, the martensitic microstructure is still puzzling, especially how it is built up in 3 dimensions. The analysis of this puzzle is complicated by grain boundaries present in polycrystalline NiTi. Here, we eliminate the influence of grain boundaries by using epitaxial NiTi films in (111)-orientation as a model system. We analyze the films with electron microscopy to identify clusters and interfaces and compare results to the phenomenological theory of martensite. With this approach, we generate a scale-bridging understanding of the martensitic microstructure. Three kinds of twin boundaries on different length scales are required for the complete, hierarchical microstructure. Integral X-ray measurements confirmed our

microstructure model. The results are transferable to NiTi bulk and polycrystalline films, showing that NiTi epitaxial films are important to extend our understanding of the martensitic microstructure.

MM 17.3 Tue 10:45 SCH A 118

Elucidating the nucleation and growth mechanism of {11-22} twin in titanium — ANDRIY OSTAPOVETS¹, ●RITU VERMA^{1,2}, and ANNA SERRA³ — ¹Institute of Physics of Materials, Czech Academy of Sciences, 616 00 Brno, Žitkova 513/22 Czech Republic — ²Central European Institute of Technology, Brno University of Technology, Purkyňova 656/123 612 00 Brno, Czech Republic — ³Universitat Politècnica de Catalunya, Campus Nord, C-2, Jordi Girona, 1-3, 08034 Barcelona, Spain

{11-22} Twin is the predominant twinning mode in hcp metals such as Ti, Zr and Mg under $\langle c \rangle$ axis compression. We analyze the {11-22} twin nucleation in Ti by reverse α - ω - α phase transformation. The twin nucleated by this mechanism can grow by the migration of the {11-22} twin boundary. This migration is mediated by the gliding of line defects with step and dislocation character, i.e. $b_3/3$ disconnection, along with {11-22} twin boundary. Their structure can be interpreted as a pair of disconnections (bt and bt*) i.e. dissociated core of $b_3/3$ disconnection, which contains ω -phase structure inside. These studies reveal the role of ω -phase in the connection with nucleation and growth mechanism of {11-22} twin boundary. These results clarify the uncertainties with the growth of the {11-22} twins.

MM 17.4 Tue 11:00 SCH A 118

Bicontinuous microstructure formation through peritectic melting — ●ZHONGYANG LI¹, NINA PETERSEN¹, LUKAS LÜHRS¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg — ²Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht

Recent research has found that when heated above the peritectic line, the intermetallic compound TiAg decomposes into a separated solid Ti phase and a liquid Ag phase, thereby forming a bicontinuous microstructure. This shows that monolithic networks such as porous Titanium, which has potential application in the field of biomedicine, can be produced with simple heat treatment followed by selective removal of other phases. As a novel dealloying method for bulk materials, the underlying mechanism is still not completely understood. It is also unclear if this method could be used in different alloy systems.

In our research we find a similar microstructural phenomenon for CuSn alloys. With the help of electron microscopy and X-Ray diffraction, formation and evolution processes of the bicontinuous structure of both TiAg and CuSn systems are studied. Research on microstructure evolution can help both, setting up the criteria for searching new alloy systems and optimizing thermal treatment parameters. This enables us to further develop this method for porous metal preparation, and also broaden the application of this method from peritectic dealloying to dealloying at crystal-melt coexistence.

MM 18: Transport in Materials: Metals, Alloys and Oxides

Time: Tuesday 11:30–13:00

Location: SCH A 118

MM 18.1 Tue 11:30 SCH A 118

Understanding diffusion in high entropy alloys from an experiment-ab initio approach — ●XI ZHANG¹, SERGIY DIVINSKI², and BLAZEJ GRABOWSKI¹ — ¹Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany — ²Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Diffusion in high entropy alloys (HEAs), due to the significant chemical complexity and the severe lattice distortion, has many fundamental features that are extremely important for both basic research and industrial development. The most accurate and direct method to study diffusion is the radiotracer technique whereby a number of intriguing phenomena, e.g., ultra-fast, non-/anti-sluggish diffusion, have been observed. To advance the current understanding of the observed phenomena, accurate theoretical analysis is highly required. The key point of the present approach is the combined measurement of diffusivities and interdiffusion profiles on the one hand and a highly accurate DFT-informed assessment of the diffusion mechanisms on the other. In this way, the long-standing mysteries in HEA diffusion, e.g., "sluggish" diffusion, can be comprehensively examined and understood. Remarkably, we show by investigating an HCP AlScHfTiZr HEA system that the increasing chemical complexity results in a considerably broadened distribution of the defect formation and migration energies which may enhance the mobility of the defects and thus the diffusion rates. The observed "anti-sluggish" diffusion can be traced back to the lattice distortion as revealed by the DFT calculations.

MM 18.2 Tue 11:45 SCH A 118

Composition dependent thermodynamic factor, Manning factor, and impurity diffusion coefficients estimated by a tracer-interdiffusion couple technique — ●ESAKKIRAJA NEELAMEGAN¹, DANIEL GAERTNER¹, JASPER BERNDT², STEPHAN KLEMME², ALOKE PAUL³, GERHARD WILDE¹, and SERGIY V DIVINSKI¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Institut für Mineralogie, University of Münster, Münster, Germany — ³Department of Materials Engineering, Indian Institute of Science, Bangalore, India

The thermodynamic driving force for the diffusion was never validated experimentally. The newly proposed augmented tracer-interdiffusion couple method could be adapted to validate the thermodynamic factor. The approach is demonstrated for a model Ni-Fe binary system, especially for the Ni-rich corner. Pure Ni is diffusion-coupled with a Ni-10 at. % Fe diluted alloy at 1000 C for 24h. The interdiffusion coefficients are estimated from the composition profile measured by an Electron Microprobe Analyser. The composition-dependent tracer diffusion coefficients are estimated following the Belova-Murch approach. Diffusion of the Fe55 and Ni63 isotopes under a chemical gradient is followed. The Fe tracer diffusion coefficients are found to be faster than those of Ni in this composition region. Utilizing the Darken-Manning relation, the thermodynamic factor is estimated and compared with that provided by a ThermoCalc software database. As a result, the composition-dependent impurity diffusion coefficients of Co, Cr, and Mn in these alloys are analysed in detail.

MM 18.3 Tue 12:00 SCH A 118

Control of microstructure in binary alloy thin films by means of electromigration — ●THOMAS BREDE, REINER KIRCHHEIM, and CYNTHIA A. VOLKERT — Universität Göttingen, Institut für Materialphysik, Göttingen, Deutschland

Magnetic and electric fields and currents open new and efficient materials processing paths for microstructure optimization than were previously available. For example, it has recently been shown that high DC electric currents can be used to create anisotropic microstructures with elongated ferrite grains in iron-carbon thin films [1]. The elongated grains form in the wake of carbides that migrate due to electromigration induced carbon flux divergences. The underlying mechanisms controlling the microstructural evolution will be presented and will be used to discuss other materials systems that might show this effect and how they could be implemented to achieve precise microstructure control.

[1] Brede, T., Kirchheim, R., & Volkert, C. A. (2020). Anisotropic grain growth in iron-carbon films at high electric current densities. *Scripta Materialia*, 178, 18-23.

MM 18.4 Tue 12:15 SCH A 118

GP-zone formation and growth in rapidly quenched Al-Cu alloys — ●DAVID STEIN, JOHANNES BERLIN, TOBIAS STEGMÜLLER, and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, 86159 Augsburg, Germany

Natural aging by the formation of Guinier Preston zones in Al-Cu alloys is only possible in the presence of excess vacancies, quenched in from high temperatures. In collision welded samples of Al and Cu, an unexpected high density of GP-zones was observed in the TEM. In order to obtain similarly high quenching rates of about 104 K/s, meltspinning was used for alloys with a Cu content from 2-5 wt%. After the quenching process, the samples were analyzed after different natural aging times using Differential Scanning Calometry (DSC), hardness measurements, resistometry and STEM to obtain information about the unmixing kinetics. Additionally EDX and EBSD were used to characterize the microstructure and chemical homogeneity of the samples.

MM 18.5 Tue 12:30 SCH A 118

Theoretical studies on the oxygen migration through crystalline strontium titanate — ●CARMEN FUCHS¹ and TIMO JACOB^{1,2,3} — ¹Ulm University, Institute of Electrochemistry, D-89069 Ulm — ²Helmholtz-Institute-Ulm (HIU), D-89081 Ulm — ³Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe

Transition metal oxides with perovskite structure (ABO₃) display a range of complex physical phenomena of condensed matter physics, including superconductivity, ferroelectricity, and magnetism. Strontium titanate, SrTiO₃ (STO), is the archetypical and most frequently studied representative of perovskite materials. By changing the stoichiometry, major changes in several important properties can be induced including blue light emission,[1] local conductivity,[2] and electron doping.[3] The relationship between the structure and the diffusion behavior of defects in SrTiO₃ is studied via DFT calculations using the plane-augmented wave method and the PBE exchange-correlation functional with and without Hubbard U correction. The obtained defect formation energy and activation barriers for oxygen migration through Frenkel- and Schottky-like defects within the crystalline STO structure are discussed and summarized. [1] D. Kan et al, *Nat. Mater.* 4 (2005), 816-819. [2] K. Szot, W. Speier, G. Bihlmayer, R. Waser, *Nat. Mater.* 5 (2006), 312-320. [3] A.F. Santander-Syro et al, *Nature* 469 (2011), 189-193.

MM 18.6 Tue 12:45 SCH A 118

Impact of alloying elements on point defects and diffusion in B2 alloys: an ab initio study — ●ADITYA VISHWAKARMA¹, OSAMU WASEDA¹, TILMANN HICKEL¹, NEELAMEGAN ESAKKIRAJA², SERGIY DIVINSKI², and ALOKE PAUL³ — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²Institute of Materials Physics, University of Münster, Germany — ³Department of Materials Engineering, IISc Bangalore, India

Turbine blades in jet engines are vulnerable to many problems due to the harsh application environments. To prevent oxidation and surface degradation, bond coats of B2 NiAl are most widely used. During the operation at high temperatures, however, the Al content in the bond coat is lost by the formation of an Inter Diffusion Zone (IDZ) between the superalloy (turbine blade) and the bond coat. In this report, ab-initio based studies of point defect formation and kinetics are performed, in order to investigate the diffusion mechanisms and the impact of alloying elements on diffusion in B2 NiAl phase. Our results show that isoelectronic substitutions by Pt and Pd decreases the triple defect migration barriers and increases the Ni vacancy concentration in comparison to pure B2 NiAl. Accordingly, the contribution of the triple defect mechanism increases down the periodic table. These results explain the experimentally observed increase of the thickness of IDZ compared to binary B2 NiAl and have, therewith, an impact on the future design of turbine blades.

MM 19: Development of Computational Methods: Simulation Methods – Theory

Time: Tuesday 14:15–15:30

Location: SCH A 251

MM 19.1 Tue 14:15 SCH A 251

Multi-methodological study of temperature trends in Mössbauer effect in beta-Sn — •MARTIN FRIÁK¹, NIKOLAS MASNIČÁK¹, OLDŘICH SCHNEWEISS¹, PAVLA ROUPCOVÁ¹, ALENA MICHALCOVÁ², ŠÁRKA MSALLAMOVÁ², and MOJMÍR ŠOB^{3,1} — ¹Institute of Physics of Materials, Czech Academy of Science, Brno, CZ — ²Department of Metals and Corrosion Engineering, University of Chemistry and Technology in Prague, Prague, CZ — ³Department of Chemistry, Faculty of Science, Masaryk University, Brno, CZ

We have performed a multi-methodological theoretical study of impact of thermal vibrations on the Mössbauer effect in the tetragonal beta-phase of tin. We have seamlessly combined (i) atomic-scale numerical data in the form of mean square displacements of Sn atoms determined by quantum-mechanical calculations, (ii) continuum-level thermodynamic modeling based on the quasi-harmonic approximation and (iii) theoretical analysis of Mössbauer effect resulting in the prediction of temperature dependence of Mössbauer factor. The computed results were compared with our Mössbauer and X-ray experimental data. We show that classical theoretical approaches based on simplistic Debye model of thermal vibrations of solids can be nowadays replaced by exact ab initio calculations of individual thermal vibrations. For details see M. Friák at al., *Computational Materials Science* 215 (2022) 111780, doi:10.1016/j.commatsci.2022.111780.

MM 19.2 Tue 14:30 SCH A 251

Increasing the Diversity of One-Sided Transition State Searches with Biasing Potentials — •NILS GÖNNHEIMER, KING CHUN LAI, KARSTEN REUTER, and JOHANNES T. MARGRAF — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Chemical processes on catalytic surfaces are commonly described in terms of complex networks of chemical reactions. One-sided transition state (TS) searches are a powerful tool for exploring these networks, when not all reactants, products and intermediates are known. To this end, the dimer method is commonly used, since it avoids the computationally demanding calculation of second derivatives. However, a prominent disadvantage of the dimer method is the convergence to the same few TSs even with differently initialised simulations, which raises the possibility of overlooking reaction pathways. Here, we propose a method to overcome this limitation. Specifically, we use a biasing potential to modify the potential energy surface (PES) based on information gathered from previous calculations. This biasing potential is adaptively generated in a series of dimer searches to drive the searching algorithm away from already known TSs. Intuitively, such potentials can be built within the Cartesian space by placing an energy bias at the atomic positions of a found TS. Alternatively, a similarity kernel between the structure and the known TS based on a local environment descriptor can be employed. This ensures that the biasing potential is invariant to permutations between identical atoms, as well as rotations and translations. The performance of both approaches is discussed for adatom diffusion and island formation on the Pd(100) surface.

MM 19.3 Tue 14:45 SCH A 251

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 ex-

pensive 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.

MM 19.4 Tue 15:00 SCH A 251

Automated Wannierizations — •JUNFENG QIAO^{1,2}, GIOVANNI PIZZI^{1,2,3}, and NICOLA MARZARI^{1,2,3} — ¹THEOS, EPFL — ²NCCR MARVEL — ³LMS, Paul Scherrer Institut

Maximally localized Wannier functions (MLWFs) are widely used in computational condensed matter physics. The standard approach to construct MLWFs often requires initial guesses which are based on chemical intuition and some measure of trial and error. Here, we first introduce an algorithm based on “projectability disentanglement” that provides reliably and automatically atom-centered Wannier functions describing both occupied and empty states. Then, we show how to mix these again into target subspaces; e.g., to describe valence and conduction bands separately. We test these algorithms on 200 representative materials (77 insulators), showing that the final MLWFs are very well localized and can accurately interpolate band structures at the meV scale. Such approaches enable automated Wannierizations for both metals and insulators, promoting further applications of MLWFs in physical applications and high-throughput calculations.

MM 19.5 Tue 15:15 SCH A 251

Higher-order finite difference method for accurate calculation of Wannier centers and position matrix elements — •MINSU GHIM^{1,2,3}, JAE-MO LIHM^{1,2,3}, and CHEOL-HWAN PARK^{1,2,3} — ¹Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — ²Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — ³Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

An accurate calculation of Wannier function centers and position matrix elements is crucial for calculating many physical quantities such as the electric polarization and optical responses from first-principles Wannier interpolation. Since the Fourier transform of the position operator is the gradient in momentum space, a finite difference technique is used to calculate the position matrix elements for Wannier functions. However, so far, only the first-order finite difference has been considered therein. We present a higher-order finite difference method and demonstrate the advantage of our method over the conventional first-order finite difference method.

MM 20: Topical Session: Fundamentals of Fracture – Microstructure Impact on Fracture (Experiments)

Time: Tuesday 14:15–15:30

Location: SCH A 216

MM 20.1 Tue 14:15 SCH A 216

Fatigue damage prediction using graph neural networks on microstructure representations — ●ALI RIZA DURMAZ^{1,2,3}, AKHIL THOMAS^{1,2}, CHRIS EBERL^{1,2}, and PETER GUMBSCH^{1,3} — ¹Fraunhofer Institute for Mechanics of Materials IWM, Freiburg im Breisgau, Germany — ²University of Freiburg, Freiburg im Breisgau, Germany — ³Karlsruhe Institute of Technology, Karlsruhe, Germany

Crack initiation governs high-cycle fatigue (HCF) life and makes HCF very susceptible to microstructural details. Predicting microscopic cyclic plasticity in polycrystals requires thorough microstructure representations.

In this work, we compare phenomenological crystal plasticity models with graph machine learning models on the task of predicting local cyclic plasticity in ferritic steel (EN1.4003). A workflow is presented which consists of a combined experimental and data post-processing pipeline to establish fatigue damage/crack initiation and short crack propagation data sets efficiently. It evolves around fatigue testing of mesoscale specimens to increase damage detection sensitivity, data fusion through multi-modal registration to address data heterogeneity, and image-based data-driven damage localization. The resulting data fuels both crystal plasticity and graph machine learning efforts. For the latter, the pixel data is transcribed into graph representations of the microstructure before being fed to different graph neural network variants. Interpretability techniques are applied to the machine learning models to learn about driving forces for the formation of extrusions and protrusions in individual grains.

MM 20.2 Tue 14:30 SCH A 216

analysis of plasticity in cyclic compression precracking — ●MOHAMED AMINE FAHAM, NATHALIE LIMODIN, JEAN FRANÇOIS WITZ, and JÉRÔME HOSDEZ — Univ. Lille, CNRS, Centrale Lille, UMR 9013 - LaMcube - Laboratoire de Mécanique, Multiphysique, Multiéchelle, F-59000 Lille, France

Determining whether a defect will grow or not is of utmost importance particularly for railway axles. In this context, compressive precracking is an interesting procedure to get fatigue crack growth threshold. Using this method, specimens are precracked with both maximum and minimum compressive loads. This study uses fracture mechanics analysis, digital image correlation (DIC) and finite element method (FEM) to assess compressive plastic zone and precrack length ahead of a SENT specimen notch.

The DIC strain field in the direction of loading shows the evolution of the monotonic compressive zone ahead of the notch with increasing load. Other techniques were used to assess the plasticity ahead of the notch and to verify DIC vertical strain field results. One technique consists of projecting (in the least squares sense) the measured DIC displacement fields on Williams' basis. The difference between the DIC vertical displacement field and the analytical one highlights the plasticity in the notch region. A coupled DIC-FEM simulation with boundary conditions issued from DIC displacement fields applied on a numerical model of the specimen with inelastic material behavior was done in order to verify the extent of the compressive plastic zone and to estimate the compressive precrack length.

MM 20.3 Tue 14:45 SCH A 216

Microstructural damage analysis in a DP800 steel subjected to complex strain paths — ●MAXIMILIAN A. WOLLENWEBER, LUIZ R. GUIMARÃES, NICOLE LOHREY, SETAREH MEDGHALCHI, TALAL AL-SAMMAN, and SANDRA KORTE-KERZEL — RWTH Aachen, Aachen, Germany

During forming processes, initiation and evolution of microstructural damage sites have a strong negative influence on the mechanical prop-

erties of the finished product. It is therefore important to investigate the damage behavior during deformation and unravel its relationship with the strain path. The current work investigates the microscopic damage evolution in a dual-phase steel DP800 subjected to different loading scenarios in tension and bending. The aim is to elucidate how the strain path influences the initiation and growth of microstructural damage in order to design more damage-tolerant industrial forming processes. The methods used comprise machine-learning algorithms and in-situ testing in a scanning electron microscope to observe and classify damage sites in the deformed samples. The results show that strain hardening inhibits damage formation, while pre-existing damage sites tend to facilitate further damage formation.

MM 20.4 Tue 15:00 SCH A 216

Three-dimensional characterization of damage sites and strain dependence in dual phase steel — ●SETAREH MEDGHALCHI¹, BINBIN LIN², JOSCHA KORTMANN¹, BAI-XIANG XU², ULRICH KERZEL³, and SANDRA KORTE-KERZEL¹ — ¹Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Aachen, Germany — ²Mechanics of Functional Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany — ³Fakultät für Georesourcen und Materialtechnik, RWTH Aachen University, Aachen, Germany

High performance materials like dual phase steels possess a heterogeneous microstructure resulting in the unique interplay between the two phases. High resolution scanning electron microscopy serves as a tool to unravel many of the microscale properties related to the deformation and mechanical properties of these materials. Damage sites in the microstructure serve as the main controlling feature during deformation. There are two fronts to tackle for a deeper understanding of the global damage accumulation: First, bringing high resolution analysis to large scales, and second, moving from two dimensional to three-dimensional characterization. We approach this challenge by employing slice-and-view SEM sectioning in combination with automated convolutional neural networks. With the knowledge of the damage occurring in different positions with various local conditions, we combine some related parameters to capture not only the trajectory of the damage sites inside the volume of the sample, but also the relative local stress-strain distribution condition.

MM 20.5 Tue 15:15 SCH A 216

Experimental and computational crack growth analysis under in-phase and out-of-phase thermo-mechanical fatigue — ●VALERY SHLYANNIKOV, ALEKSANDR SULAMANIDZE, and DMITRY KOISOV — Kazan, Russia

This study presents interpretation and evaluation of non-isothermal experimental crack growth data generated by tests carrying out by stress-controlled in-phase (IP) and out-of-phase (OOP) thermo-mechanical fatigue (TMF) conditions. A crack growth testing method has been developed utilizing inductive heating and direct the crack tip opening displacement (CTOD) techniques for polycrystalline XH73M nickel-based alloy. The crack growth experimental results interpretation is based on finite element analyses of the mechanical stress-strain rate fields at the crack tip and new fracture resistance parameters. To this end, an algorithm for multi-physics numerical calculations was developed and implemented by incorporating Maxwell 3D, Fluent, and the transient structural modules of ANSYS 2021R1, to understand the mechanics of crack tip deformation under thermo-mechanical loading conditions. Fatigue fracture diagrams build in terms of new crack growth parameters have shown that in-phase testing produces accelerated crack growth rates compared with out-of-phase due to increased temperature at peak stress and therefore increased time dependent crack growth.

MM 21: Materials for Storage and Conversion of Energy: Energy Conversion

Time: Tuesday 14:15–15:30

Location: SCH A 215

MM 21.1 Tue 14:15 SCH A 215

Harvesting of low-grade waste heat with shape memory alloys — ●BRUNO NEUMANN^{1,2} and SEBASTIAN FÄHLER¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf — ²Technische Universität Dresden

More than half of all energy converted by humankind is lost in the form of waste heat. Not only does that strongly contribute to the acceleration of global warming, it also leaves an enormous economic potential untouched. However, suitable technologies are limited, since most of this heat is of low temperature (< 100 °C). In the last years, materials and technologies for thermoelectric harvesting and thermomagnetic harvesting have been explored, but a high efficiency of those systems remain a challenge. With our work, we present a thermoelastic harvesting approach for converting the waste heat of a fluid into electricity, utilizing shape memory alloy wires. These wires bring the inherent advantage that their transformation temperatures can be adapted to the required temperature range of the waste heat. Moreover, they provide a very high actuation energy density and are commercially available. In our set-up, we use two mechanically connected arrays of wires to reach a high power density of the system. Our simulation data predicts a thermodynamic efficiency in respect to the Carnot efficiency of 22.7 %, which exceeds current efficiency benchmarks set by thermoelectric materials.

MM 21.2 Tue 14:30 SCH A 215

Atomistic simulations of the Seebeck effect in electrolytes — ●OLE NICKEL¹, MATHIJS JANSSEN², and ROBERT MEISSNER¹ — ¹Hamburg University of Technology, Hamburg, Germany — ²University of Oslo, Oslo, Norway

The Seebeck effect allows electrical energy to be obtained directly from thermal gradients. In electrolytes it is based on an differential heat of transport of the ions.

We perform molecular dynamic simulations with different electrolytes between graphene electrodes. We apply an external resistance between the electrodes via a thermopotentiostat, where the thermal fluctuation term is deactivated, effectively resembling an RC-circuit with a time constant of $\tau=RC$.

With this method it is possible to simulate a complete electrochemical cell in open circuit conditions which is charged with a thermal gradient and then discharged at constant temperature. The Seebeck energy is the energy that is dissipated across the external resistance. The goal is to investigate optimal electrolyte parameters to maximize this energy.

MM 21.3 Tue 14:45 SCH A 215

Non-Local DFT calculations towards the discovery of stable water-splitting catalysts — ●AKHIL S. NAIR, LUCAS FOPPA, EVGENY MOERMAN, and MATTHIAS SCHEFFLER — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin, Germany

Efficient prediction of the thermodynamic and aqueous stability of materials is essential for leveraging the catalyst discovery for the water splitting reaction. In particular, the oxygen evolution half-reaction is

usually carried out using oxide catalysts under harsh potential and pH conditions.[1] This necessitates the application of DFT methods which can predict the oxide stability under experimentally relevant conditions without any *ad hoc* corrections.[2] In this regard, herein, we employ a non-local DFT method using the hybrid HSE functional for calculating the stability of oxide catalysts. Crucially, we scrutinize the effect of the HSE mixing parameter on the formation energies and aqueous stability of oxides and compare to higher-level calculations using coupled-cluster theory for reference systems. Through this approach, we attempt to standardize the application of HSE method for accurate oxide stability prediction which could augment the large-scale catalyst discovery.

[1] Z.Wang, *et al.*, *npj Comput. Mater.* **6**, 160 (2020).

[2] L.-F. Huang, J. M. Rondinelli, *npj Mater. Degrad.* **3**, 26 (2019).

MM 21.4 Tue 15:00 SCH A 215

Photocatalytic water splitting from Koopmans spectral functionals: The case of TiO_2 polymorphs — ●MARIJA STOJKOVIC¹, EDWARD LINSKOTT¹, and NICOLA MARZARI^{1,2} — ¹Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — ²Laboratory for Materials Simulations, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Photocatalytic water splitting has drawn considerable attention for renewable energy production. Since the first reported photocatalytic water splitting by titanium dioxide, this material remains one of the most promising photocatalysts, due to its suitable band gap and band-edge positions. However, estimating both of these properties is a challenging task for standard DFT functionals. Here we show how Koopmans spectral functionals can accurately predict the band structure and level alignment of rutile, anatase and brookite, demonstrating the advantage of orbital-density dependent functionals for predicting the spectral properties of materials.

MM 21.5 Tue 15:15 SCH A 215

DFTB Description of the Ground and Excited States Properties of Thiolate Protected Gold Nanoclusters — ●CARLOS R. LIEN-MEDRANO¹, ARNAUD FIHEY², and THOMAS FRAUENHEIM¹ — ¹University of Bremen, Bremen, Germany — ²University of Rennes, Rennes, France

Gold nanoclusters stand as promising building blocks for solar energy harvesting applications, luminescent materials and catalytic devices. At the frontier between molecular and metallic structures, their large number of electrons prevent the use of *ab initio* quantum mechanic method to rationalize and predict their structure-property relationships, especially when fully coated with organic ligands. Using a semi-empirical DFT-based scheme, namely Tight-Binding Density Functional (DFTB), we demonstrate that it is possible to rapidly access the ground (geometry and electronic structure) and excited state (UV-Visible absorption) properties of these nano-objects without sacrificing the qualitative accuracy of its parent DFT, paving the way towards a quantum material design of gold-organic nano-devices.

MM 22: Mechanical Properties and Alloy Design: Porous and Nanostructured Materials

Time: Tuesday 14:15–15:45

Location: SCH A 118

MM 22.1 Tue 14:15 SCH A 118

tailoring mechanical properties of lightweight 1D Nanostructures — SAMUEL BALTAZAR^{1,2}, JAVIER ROJAS^{1,2}, ●FELIPE VALENCIA^{2,3}, SEBASTIAN ALLENDE^{1,2}, RAFAEL GONZALEZ^{2,4}, EDUARDO BRINGA⁵, and PIERRE COCCO-MAGNARD² — ¹Physics Department, Universidad de Santiago de Chile, Chile — ²Center for the development of Nanoscience and Nanotechnology, Universidad de Santiago de Chile, Chile — ³Engineering Faculty, Universidad Catolica del Maule, Chile — ⁴Centro de Nanotecnología Aplicada, Universidad Mayor, Chile — ⁵CONICET & Facultad de Ingeniería, Universidad de Mendoza, Argentina

1D Nanostructures such as nanowires (NW) and nanotubes (NT) have gained a lot of attention due to their mechanical and electronic properties. The deformation of NT and NW has been previously studied, finding different fracture mechanisms. Tension and compression deformations show elastic regimes until a sudden stress drop due to the fast generation of dislocations. Synthesis of polycrystalline NW allows the reinforcement of the material's response. We report the mechanical properties are studied for mono and bimetallic systems by means of molecular dynamics simulations. Interatomic potentials were used to model Ni, Fe, and bimetallic NTs and NWs with dimensions similar to the experimental setup. Ni NT shows an asymmetry in the stress response under tension and compression, mediated by twins and stacking-faults dislocations, with no significant degradation of mechanical properties up to 60% mass reduction than NW, opening the generation of new lightweight and resistant materials.

MM 22.2 Tue 14:30 SCH A 118

Comparing structural response of filled and porous 3D Titanium network structures by application of nanotomography and graph theory — ●STEFAN A. BERGER¹, MARKUS ZIEHMER¹, and JÜRGEN MARKMANN^{1,2} — ¹Helmholtz Zentrum Hereon — ²Technische Universität Hamburg

Recently, refinements of the classical Gibson-Ashby relation have been invoked to extend its applicability to the description of the mechanical properties of bicontinuous, nanoporous metals. In particular, the network connectivity has been identified as a crucial parameter that needs to be taken under consideration. So far, global parameters like connectivity or genus (density) have been employed. However, these do not uniquely identify the underlying microstructure. This can be achieved by making use of graph theoretical aspects, as demonstrated in Ziehmer et al[1]. In this work, we have investigated the changes in the network structures of porous Titanium and Ti-Mg composites, fabricated by Liquid Metal Dealloying, during compression tests in a x-ray nanotomograph. The reconstructed sample volumes were simplified by skeletonization, the resulting skeletons transferred into a weighted graph representation, and further decomposed into the constituent rings that built the network. This approach allowed for a statistical description of the behavior of the ring elements under load. One major result is that the essential part of deformation is carried by larger rings. [1] M. Ziehmer, E. T. Lilleodden, Acta Materialia 199 (2020).

MM 22.3 Tue 14:45 SCH A 118

Hierarchical-structural effects on mechanical behavior of nanoporous gold in electrochemical environment — ●HANSOL JEON¹, SHAN SHI^{3,1}, and JÜRGEN MARKMANN^{1,2} — ¹Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — ²Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — ³Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany

Recently, hierarchical nanoporous gold (HNPG) has been emerged with having multiple-level structures. HNPG is more active because of higher surface area than nanoporous gold (NPG) since Au ligaments are supposed to be converted into another porous structure with smaller ligaments and pores. Regarding mechanical behavior, especially with the same solid fraction for both, it has been not directly compared yet whether HNPG would have better mechanical properties. Here, we investigated the mechanical properties of NPG and HNPG with the same solid fraction by conducting compressive tests at the micro-scale. The NPG and HNPG were prepared from the

same precursor alloy Ag85Au15 by dealloying. The pillars were milled by a focused ion beam (FIB), and compressive tests were performed by a nanoindenter with a flat-punch tip. We discussed the difference of dislocation activities and connectivity for NPG and HNPG. Finally, by conducting additional compressive tests in an electrochemical environment, we explored the role of surface state on the mechanical behavior of NPG and HNPG by imposing electrode potential.

MM 22.4 Tue 15:00 SCH A 118

Mechanical properties and oxidation performance of nanostructured self-passivating WCrY material — ●JIE CHEN¹, ANDREY LITNOVSKY¹, JESUS GONZALEZ-JULIAN^{1,2}, JAN WILLEM COENEN¹, and CHRISTIAN LINSMEIER¹ — ¹Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany — ²Institute of Mineral Engineering, RWTH Aachen University, 52074 Aachen, Germany

Self-passivating W-11.4wt%-0.6wt%Y alloy have been considered as a promising plasma-facing material in fusion power plants. In the present work, bulk material are fabricated via holding at 1300C for 2 minutes in field-assisted sintering. As a result, an average matrix's grain size of 98.9nm and 6.7% surface area of Cr-rich phase was obtained. Cr-rich phase is formed on the surface of particles during sintering and over 70 at% of Cr is detected by EDX. A hardness HV0.5 of 1287.6 is obtained as a result of small grains while a fraction of Cr-rich phase in the microstructure softens material to some extent. Three point bending tests at temperature up to 1000C are performed to measure fracture toughness and ductile brittle transition temperature. This is done combining with fractography study to investigate the effect of grain size as well as Cr-rich phase on the thermo-mechanical properties. Reduction in grain size down to the order of sub-micrometer range is proven to improve material's anti-oxidation performance in previous study. Oxidation test was performed at 1000C to investigate performance of the microstructure developed. Details of the work are presented in this contribution.

MM 22.5 Tue 15:15 SCH A 118

Study of the oxidation mechanism of Cr₂AlC MAX phase through nanoscale analysis of alumina scale formation — ●ANICHA REUBAN^{1,2}, JESUS GONZALEZ-JULIAN^{1,2}, IVAN POVSTUGAR¹, ANDREY LITNOVSKY¹, and CHRISTIAN LINSMEIER¹ — ¹Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — ²Institute of Mineral Engineering, RWTH Aachen University, 52074 Aachen, Germany

In a Concentrated Solar Power (CSP) plant, the receiver must withstand temperatures >800 °C, be resistant to oxidation by air and/or corrosion by molten salts and maintain its properties over time. MAX phases, which are ternary carbides and nitrides with a unique combination of ceramic and metallic properties, are candidate materials for the receiver. In this work, the oxidation mechanism of the alumina-forming MAX phase Chromium Aluminium Carbide (Cr₂AlC) is studied. The samples are oxidized in a thermogravimetric analyzer (TGA) at 1000 °C and 1200 °C in humid air. The oxide scale is characterized using XRD, FIB-SEM, EDX and STEM. The alpha alumina layer formed consists of needle-like grains on top, with larger grains at the bottom, below which is a layer of chromium carbide. The elemental distribution across grain boundaries and interfaces of various regions of the oxide scale, carbide and bulk material are being analyzed with Atom Probe Tomography (APT), since these are possible pathways for the diffusion of aluminium and oxygen ions to form the oxide layer. The effect of dissolved chromium in the oxide scale and the segregation of impurities such as iron and silicon to interfaces is examined.

MM 22.6 Tue 15:30 SCH A 118

Phase stability of iron and its alloys from first principles dynamical simulations and thermodynamic integration — ●DAVIDE GAMBINO and BJÖRN ALLING — Linköping University, Linköping, Sweden

In recent years, thermodynamic integration (TI) based on first principles simulations has been shown to accurately reproduce phase diagrams and is now able to guide the design of functional materials and alloys. For what concerns iron and steels, this methodology is complicated by the presence of magnetic degrees of freedom (DOF) and

their interplay with electronic and vibrational DOFs. Here I will show how the phase stability of iron and its alloys can be obtained from first principles employing atomistic spin dynamics - ab initio molecular dynamics (ASD-AIMD) simulations and TI accounting for all DOFs [1].

The free energy difference between bcc and fcc Fe was calculated close to the melting point in the magnetically disordered state, carrying out TI over stress-strain variables along the Bain path, and then propagating it to low temperatures with TI over temperature employ-

ing the ASD-AIMD energies. The method captures the $\alpha \rightarrow \gamma \rightarrow \delta$ transitions, with the latter transition temperature reproduced within 50 K from experiments, and the calculated Gibbs free energy difference being within 5 meV/atom from the CALPHAD estimate over the whole temperature range. The method is then applied to $\text{Fe}_{1-x}\text{Mn}_x$ alloys for concentrations of $x = 0.05, 0.10$ and for temperatures $T \geq 1400$ K and results are compared with the experimental phase diagram.

[1] Gambino et al., arXiv:2210.14718 [cond-mat.mtrl-sci]

MM 23: Poster II

Time: Tuesday 18:15–20:00

Location: P2/OG1+2

MM 23.1 Tue 18:15 P2/OG1+2

(ZnO) 42 Nanocluster: A Novel Visibly Active Magic Quantum Dot under First Principle Investigation — ●BIJAL MEHTA and DEBESH ROY — Materials and Biophysics Group, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India.

A systematic density functional investigation on the structural, electronic and optical properties of the growth of (ZnO) 6 cluster unit in the series of (ZnO) 6n for n=1*9 is performed in this report. Different electronic properties of (ZnO) 6n nanoclusters are analyzed in terms of HOMO-LUMO gap (HLG), ionization potential (IP), electron affinity (EA), chemical hardness (η), and electrophilicity index (ω) which all shows a zigzag behavior as the size of (ZnO) 6n clusters increases. The clusters' electronic energy gain (*E) identified an exceptionally stable *magic* nanocluster, viz. (ZnO) 42. Frontier orbitals analysis results indicate easy electron transfer in (ZnO) 42 nanocluster system. The optical absorption spectra confirm that the magic (ZnO) 42 nanocluster is active in electromagnetic radiation's visible range ($\lambda=406.8$ Å). Interestingly, similar optical switching towards the growth of (ZnO) 6 unit is also observed like zig-zag electronic properties. The simulation results of electronic properties as well as the infrared spectra of magic (ZnO) 42 cluster will open up a vista to the experimentalists for its possible synthesis, which in turn will help in the development of the visibly active magic (ZnO) 42 nanocluster with novel applications in the fields of quantum dots or assembled materials.

MM 23.2 Tue 18:15 P2/OG1+2

Investigation of the stability for AlB₂-type transition metal diborides from electronic structure — ●NEBAHAT BULUT and JENS KORTUS — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

Boron has huge chemical bonding diversity (metallic, ionic, and covalent bonds) because it provides fewer valence electrons compared to the number of orbitals it can form. Not surprisingly, intermetallic borides can crystallize in many different crystal symmetries, for example cubic, hexagonal or orthorhombic. The unit cell of the hexagonal AlB₂-type has two trigonal prisms in which borons are in the center surrounded by six metal atoms. Interestingly, not all twenty eight transition metals form the AlB₂-type crystal structure. The goal of the study is to understand the chemical bonding nature in detail in order to answer why some of these compounds are stable in AlB₂-type structure while others are not. We investigate the impact of the *d*-orbitals of the transition metals on the stability in order to provide a guideline to possible new transition metal diborides. The chemical bonding and charge transfer in these transition metal diborides is investigated by electronic structure calculations based on density functional theory as implemented in Quantum Espresso [1]. The study is focused on the analysis of the electron density together with the electron localization function (ELF) and provide thermodynamic information e.g. formation enthalpies, and mechanical properties.

[1] P. Giannozzi et al., J. Chem. Phys. 152 154105 (2020)

MM 23.3 Tue 18:15 P2/OG1+2

Trapping and detrapping of excess vacancies during natural ageing in Al-Cu — ●TOBIAS STEGMÜLLER, JOHANNES BERLIN, ANDREAS SCHUSS, and FERDINAND HAIDER — University of Augsburg, Chair for Experimental Physics I, Universitätsstr. 1, 86159 Augsburg

A special feature of Al-Cu alloys is the occurrence of decomposition in supersaturated solid solutions by the formation of Guinier-Preston zones (GPZ) even at ambient temperature, where the equilibrium diffusion coefficient is far too low for any unmixing. A condition for

this natural ageing is the existence of excess vacancies which remain in the material after quenching from the homogenisation temperature. As the ageing process proceeds for surprisingly long times (hours or days), the vacancies seem to be stabilised in the material and do not decay to the equilibrium value, which would stop the ageing.

Although there exist theories on the stabilisation of excess vacancies, there is no established and verified model to explain the effect. To illuminate the mechanisms behind the long term formation of GPZ we combine results from TEM and DSC measurements as well as Monte Carlo, molecular static and DFT simulations, which reveal that the GPZ themselves may act as temporal vacancy traps. Values for the trapping energy for vacancies in GPZ and on dislocations are estimated from simulations.

MM 23.4 Tue 18:15 P2/OG1+2

Proof of concept for micro pulling down growth of phase change materials in the example system of NiTi — ●LAURITZ SCHNATMANN, TIMON SIEWEKE, and GABI SCHIERNING — University of Bielefeld

The micro pulling down growth method (mPD) is a common approach to synthesize small crystals for material screening in e.g. high-entropy oxides. Another interesting group of materials are phase change materials namely showing unique structural transitions interplaying with electronic and magnetic contributions. However, the interplay between the different contributions is strongly dependent on the composition of materials. We built up a micro pulling down set up for fast material screening of phase changing materials. We grew a NiTi- shape memory alloy to show the possibility of comparable easy growth of crystals by mPD. Hereby, we verified mPD as a powerful tool for the versatile fabrication of small crystals in the field of phase change materials.

MM 23.5 Tue 18:15 P2/OG1+2

The role of electrons during the martensitic phase transformation in NiTi-based shape memory alloys — ●ALEXANDER KUNZMANN¹, JAN FRENZEL², ULRIKE WOLFF³, JEONG WOO HAN⁴, LARS GIEBELER³, DAVID PIORUNEK², MARTIN MITTENDORF⁴, JULIANE SCHEITER³, HEIKO REITH³, NICOLAS PEREZ³, KORNELIUS NIELSCH^{3,5}, GUNTHER EGGELER², and GABI SCHIERNING¹ — ¹Bielefeld University — ²Ruhr University Bochum — ³IFW-Dresden — ⁴University of Duisburg-Essen — ⁵TU Dresden

The present work provides an experimental contribution to the investigation of the role of conduction electrons in the martensitic phase transition of Nickel-Titanium. This material, which is structurally very well studied due to its shape memory effect, still offers room for further knowledge more than 60 years after its discovery. For this purpose, a series of alloys within the equiatomic NiTi phase was characterized by temperature-resolved transport experiments, thermodynamic characterizations and structural investigations. In addition to the well-known resistivity anomaly, a reduction of the charge carrier density by 90% was measured, which has not been described before for this class of materials. Using a novel approach for structural materials, conclusions could be drawn about the entropy of the electronic system and a correlation with the phase transition temperature could be demonstrated. The obtained data allow an interpretation as the formation of a charge carrier density wave phase, which explains both the drastic reduction of charge carriers and the large electronic entropy contribution.

MM 23.6 Tue 18:15 P2/OG1+2

developing high-hardness, high-electrical conductivity and gradient structure of bulk Al-2.5Fe alloy by a new severe plastic deformation: high pressure torsion extrusion — ●RU1

Xu — Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

The effect of High Pressure Torsion Extrusion (HPTE) on microstructure, hardness and electrical conductivity has been investigated in the bulk Al-2.5Fe alloy. The equivalent strain accumulated in the samples after one pass of HPTE varied in a wide range between 0.9 and 24.8, depending on the processing parameters. HPTE led to the formation of a gradient microstructure in which the grain and Al6Fe intermetallic size decreased by increasing the distance from the central axis of the samples. With increasing the equivalent strain, which is below 5.7, the microhardness and the electrical conductivity simultaneously increased, from 53.7 HV to 87 HV, from 38% IACS to 47% IACS respectively. This can be attributed to the grain size and Al6Fe intermetallic size decreased. When the equivalent strain gradually increased to 24.8, the microhardness continuously increased from 87 Hv to 126 Hv, the electrical conductivity decreased from 47% IACS to 43% IACS. This is contributed to the grain and Al6Fe intermetallic transformed into nanometer size, which significantly increased the microhardness, and some Fe atoms into Al matrix, which decreased the electrical conductivity. The High Pressure Torsion Extrusion process can lead to gradient microstructure and simultaneously increase the microhardness and the electrical conductivity of bulk Al-2.5Fe alloy.

MM 23.7 Tue 18:15 P2/OG1+2

In situ XRD measurements of a Si Li half battery cell — ●LEONARD AUE, FREDERIK STENDER, THOMAS BREDE, and CYNTHIA VOLKERT — Georg-August-Universität Göttingen, Deutschland

Li-ion batteries have become an indispensable part of modern life. They enable the repeated storage of energy on a medium and small scale, for example in electric vehicles or mobile devices.

In addition to the commonly used graphite, silicon is gaining increasing attention as a suitable anode material due to its higher capacity. However, this capacity decreases rapidly in application and a significant increase of the internal resistance occurs. Both are mainly caused by the large volume changes during lithium uptake and release.

In this work, we investigate the amorphization process that first starts during loading in in-situ XRD measurements of Si-Li composite materials in a half-battery setup. This will give us insight into Si phase changes under direct control of critical parameters such as charge or discharge rates. This knowledge could help to understand and control the phase transformations and thereby improve Si anode performance.

MM 23.8 Tue 18:15 P2/OG1+2

High capacity thin film battery electrodes from lithium titanate — YIJIE TAO, ●YUG JOSHI, and GUIDO SCHMITZ — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

Lithium titanium oxide is becoming an increasingly popular anode material for high-power Li-ion batteries due to their safe operating voltages and high cycle lifetime. The motivation to enhance the specific capacity of Li₄Ti₅O₁₂ (LTO) is of practical significance. In this work, reactive ion beam sputtering is used to deposit the titanium-based metal oxide thin films. A Li₂CO₃ modification is introduced by mixing it with LTO and using the composite as a target material. The deposition conditions (i.e., reactive oxygen) and annealing treatment (i.e., under air or vacuum at varying temperatures) are explored to optimize the thin films for the best possible capacity. X-ray diffraction (XRD), X-ray photoelectron (XPS) and electron diffraction (TEM) are used to unravel the chemical and structural nature of the thin films. The films were electrochemically characterized using cyclic voltammetry with a broad potential window, much wider than conventional LTO (i.e., 2.5V to 0.1 V vs Li/Li⁺, whereas conventional electrode is generally limited to a lower voltage of 1V). The optimized film shows good cyclic stability at a relatively high rate of 1 mV/s and show an astounding maximum capacity of 101.4 μAh*cm⁻²*μm⁻¹ after 50 cycles. To put this in context, conventional LTO shows theoretically 60.8 μAh*cm⁻²*μm⁻¹ and 91 μAh*cm⁻²*μm⁻¹ when cycled down to 1 V and 0.1 V vs Li/Li⁺, respectively.

MM 23.9 Tue 18:15 P2/OG1+2

high-rate and long-duration Sodium Storage Enabled by Sodiation-Driven Reconfiguration — ●YULIAN DONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Vanadium sulfides, with various crystal structures, such as VS₂, V₂S₃,

V₃S₄, V₅S₈, and VS₄ have attracted increasing attention because they could provide high theoretical specific capacity. Nevertheless, such vanadium-based sulfides frequently suffer significant mechanical pulverization during long-term cycling as a result of volume expansion caused by sodiation/desodiation, which result in severe irreversible capacity degradation, poor initial coulombic efficiency, reduced rate capability, and inappreciable cycling stability. Here, we demonstrate a carbon-free 3D micro-nano flower-like VS_x heterostructure electrode material that is synthesized by a facile hydrothermal process for SIB applications. The 3D micro-nano flower-like structure can well prevent the accumulation of nanosheets during electrochemical cycles and ensure full contact between the active material and the electrolyte. Therefore, 3D micro-nano flower-like VS_x electrode that finally achieves an ultrahigh-rate capacity (613.8 mAh/g at 10 A/g) and an ultra-long cyclability (more than 1500 cycles) by sodiation-driven reconfiguration for sodium ions batteries. This work presents a general approach for preparing super-high specific capacity and rate capacity electrode materials for further improving the SIBs performance.

MM 23.10 Tue 18:15 P2/OG1+2

Detection of Lithium in potential electrode materials — ●PATRICK KIRSCHT and HANS HOFSSÄSS — II Physikalisches Institut, Georg August Universität, Göttingen, Deutschland

Nuclear reaction analysis is used to quantify light elements such as lithium in a sample. The advantage of NRA is the isotope specific measurement of elements in a sample. In the current investigations we demonstrate the detection limits and sensitivity of a new setup for the detection of lithium via its nuclear reaction with protons p(7-Li,α)α with Q=17MeV. For this purpose an external proton beam with 2.5MeV is used. To determine the detection limit, lithium was implanted into silicon and ta-C near the surface by ultra-low energy ion implantation at 100eV. Furthermore, the depth profile and penetration depth were simulated using Imintdyn and SRIM and were compared with the measurements. For the measurement of diffusivity of lithium, the samples were baked at different temperatures. For comparison, MD simulation was performed using LAMMPS. These investigations are the starting point of measurements on graphene and biological materials like wood, which are considered for possible applications as electrode materials in batteries.

MM 23.11 Tue 18:15 P2/OG1+2

High-resolution measurement of displacement field from gold nanoparticles tracking — ●ANTOINE OLLIVIER, NICHOLAS BLANCHARD, ANTONIO PEREIRA, LOÏC VANEL, and DÖME TANGUY — Institut Lumière Matière-UMR 5306, Université Claude Bernard Lyon 1, 6 rue Ada Byron, 69622 Villeurbanne cedex

A new method has been developed to measure displacement field during a tensile test with both high resolution (~ 50 nm) and good precision (~ 1nm). This method has been applied on the reduced activation ferrite-martensitic steel Eurofer97. Gold nanoparticles are created by pulsed-laser induced dewetting of a nanofilm. This technique does not modify the structure of the steel below. Nanoparticles are then observed with a scanning electron microscope during tensile test. Their tracking allows to see displacement field *in situ*. This method is particularly adapted for locating heterogeneities in the displacement field and it could be very useful to understand how fracture appears.

MM 23.12 Tue 18:15 P2/OG1+2

Electronic Properties of Self-assembled 1D Gold Nanoparticle Chains — ●STEFAN M. SCHUPP¹, DAVID J. SCHUPP², EMIL SCHWARZ², REBECCA KÖSER², HELMUT CÖLFEN², and LUKAS SCHMIDT-MENDE¹ — ¹Department of Physics, University of Konstanz, Germany — ²Department of Chemistry, University of Konstanz, Germany

1D nanoparticle (NP) assemblies exhibit unique electronic properties due to their directional charge transport. In addition, the usage of stabilizing ligands enables a further possibility to add new functionalities and tune their conductivities. However, the assembly and characterization of 1D NP chains remains a challenge to this day. Here, we present a study on thiol-induced dipoles on gold (Au) nanoparticle surfaces which result in chain-like assemblies in solution under ambient conditions. Thereby, 1D assemblies of 40 nm Au-NPs with different shapes and thiolated ligands could be achieved. Afterwards, a developed transfer technique allows the electrical characterization of individual 1D NP chains through prefabricated gold electrodes. In this configuration, the temperature-dependent resistance of different NP assemblies is investigated to understand the underlying conduc-

tion mechanisms. With the gained knowledge it should be possible to generate 1D Au NP chains with controllable electronic conductivities for future applications.

MM 23.13 Tue 18:15 P2/OG1+2

Local hydrogen absorption in Pd nanoparticles observed with in-situ TEM — ●SVETLANA KORNEYCHUK¹, STEFAN WAGNER¹, GEORGIAN MELINTE², DARIUS ROHLER³, PHILLIPP VANA³, and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology, Karlsruhe, Germany — ²King Abdullah University of Science and Technology, Saudi Arabia — ³Institute of Physical Chemistry Georg-August-University Göttingen, Göttingen, Germany

The mechanism of the hydrogen absorption in metals is of a high interest for many areas of hydrogen technology, such as hydrogen storage, hydrogen detection and catalysis. Palladium is an ideal model system to study hydrogen absorption in metals due to its extreme affinity to hydrogen. Nanoscale systems, such as nanoparticles and thin films, are of the high interest to hydrogen technology due to their faster interaction with hydrogen. In this work, we investigate the behavior of a model system, Pd nanoparticles, in real time with in-situ H₂-gas TEM. With the special gas holder from Protochips it is possible to reach pressures up to 1 atmosphere and study the particles at elevated temperatures within the stability limit of the nanoparticles up to 200°C. We can observe initial stages of hydrogen absorption in Pd nanoparticles and local formation of PdH_x at different temperatures and pressures by using EELS. We support our observations with the in-situ strain measurements carried out with nanobeam electron diffraction. Finally, we propose a mechanism of hydrogen absorption in metallic nanoparticles based on the local PdH_x formation and strain measures at different loading conditions.

MM 23.14 Tue 18:15 P2/OG1+2

Investigation of the MoS₂ crystallization process in thin films — ●ANNIKA KORN, THOMAS BREDE, and CYNTHIA A. VOLKERT — Institut für Materialphysik, Göttingen, Germany

Crystalline transition metal dichalcogenide thin films show interesting potential in various application areas (e.g. optoelectronics and data storage). Crystallization of amorphous sputtered thin films is one way to produce large crystalline regions suitable for the application [1]. The aim of this work is to follow the structure of the thin films over the course of crystallization and to characterize them in different intermediate states. In this way, the process and properties of the transition can be studied and better understood. Specifically, various methods (XRD, SEM, EDX, XPS, AFM, TEM) will be used to analyze the microstructures and compositions of the samples. In addition, DSC and TGA will be used to directly measure the crystallization and possible decomposition processes.

[1] Krbal, Milos, et al.: Amorphous-to-Crystal Transition in Quasi-Two-Dimensional MoS₂: Implications for 2D Electronic Devices. In: ACS Applied Nano Materials 2021 4 (9), 8834-8844. DOI: 10.1021/ac-sanm.1c01504

MM 23.15 Tue 18:15 P2/OG1+2

Towards measuring fatigue-generated vacancies in thin copper films using nanoindenter creep tests — ●MY NGUYEN, THOMAS BREDE, JAN VERHOEVEN, and CYNTHIA VOLKERT — Institute for Materials Physics, Georg-August University of Göttingen

Vacancies can be created in metals during cyclic loading, however, they have been only rarely directly detected. In this study, we develop an experimental set-up to detect fatigue generated vacancies by measuring their contribution to creep deformation. Our methodology involves performing nanoindenter creep tests on thin metal films while they are being fatigued by cyclic loading. The fatigue is realized using delay line structures, with thin copper films on top, on which standing surface acoustic waves are generated. Contributions from thermal drift during the creep tests have been minimized using a continuous stiffness measurement method.

MM 23.16 Tue 18:15 P2/OG1+2

Optical Modulation and Phase Distribution in LiCoO₂ upon Li-ion De/Intercalation — SANAZ BANIFARSI, ●YUG JOSHI, ROBERT LAWITZKI, GÁBOR CSISZÁR, and GUIDO SCHMITZ — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

The optical modulation of sputter deposited thin-films of LiCoO₂ upon de-/lithiation is probed in reflectance geometry. The thin-films of

LiCoO₂ (LCO) are sputter-coated using ion-beam sputtering, onto mirror-like platinum current collectors. A reversible electrochemical and electrochromic behavior is obtained from the in-operando electrochemical and optical measurements. The optical constants (using ex-situ optical spectroscopy) are obtained by modelling the obtained spectra using Clausius-Mossotti relation. The model parameters reveal a dominant resonant wavelength at 646 nm for the fully intercalated LCO. For the delithiated state, Li_{0.5}CoO₂, a much broader and more intense absorption peak is obtained. This broad and intense peak is correlated to the conducting nature of the delithiated state. The obtained complex refractive index (CRI) are justified by prior reported calculations of the density of states. With the evolving CRI, the variation in the imaginary and real part of the dielectric constant is understood by a layered phase propagation. This is due to (i) the faster diffusion between the layers of CoO₆ octahedra of the layered structured LCO and, (ii) the alignment of these octahedral planes almost perpendicular to surface of the electrode as a result of the identified growth texture (due to the deposition and the subsequent annealing).

MM 23.17 Tue 18:15 P2/OG1+2

Simulations of two-dimensional amorphous materials based on force fields and ab initio calculations — ●EMEL GURBUZ and BIPLAB SANYAL — Uppsala University, Uppsala, Sweden

In recent times, low dimensional crystalline structures and van der Waals(vdW) solids have attracted a lot of attention for their huge potential in device applications. However, the exploration of two-dimensional(2D) amorphous forms is less explored. Here, we present a detailed study of structural, electronic and thermal properties of 2D amorphous graphene(A-Gra), silicene(A-Si) and silicon carbide(A-SiC) by Classical Molecular Dynamics (CMD) simulations for structure generation, stability tests, thermal conductivity and vibrational analysis along with density functional theory (DFT) calculations for the electronic structure. We find that A-Gra is planar and metallic with a thermal conductivity around 55.30 W/Km whereas the monolayer A-Si has a much lower thermal conductivity (2.68 W/Km). Among our studied materials, A-SiC's thermal conductivity is found to be the highest (70.29 W/Km). Vibrational analysis shows that the heat carriers in A-Si and A-SiC are extendons, especially diffusions in the absence of localized vibrational modes. Bilayer and trilayer structures of amorphous structures resulted respectively, in vdW bonding of A-Gra layers; covalent bonding of A-Si layers and weak bonding of SiC layers through only Si atoms. Finally, the observed uneven charge distributions can lead to the designing future electronic devices by tuning the local functionalities of 2D-amorphous structures.

MM 23.18 Tue 18:15 P2/OG1+2

Effect of micro-alloying and structural relaxation on the nanoindentation behavior of Pd-based metallic glasses — ●RICHARD VON DESTINON, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

Two methods rising in interest to modify the mechanical properties of metallic glasses consist of micro-alloying as well as relaxation. We study the influence of structural relaxation and 1 at.% additions of Fe or Co on the well-researched metallic glass Pd₄₀Ni₄₀P₂₀. The relaxation states are created by quenching from temperatures above T_g with different cooling rates. The samples are analyzed using nanoindentation with force ranges up to 1 mN. Correlations between the change in mechanical properties, such as hardness and young's modulus, and the shear deformation behavior through the pop-in distribution are investigated in detail. The results indicate that both, micro-alloying and relaxation increase the hardness of the material significantly, while the pop-in frequency remains insensitive to either.

MM 23.19 Tue 18:15 P2/OG1+2

Orientation-tunable Rod-shaped Liquid Crystal Under Surface Acoustic Wave — ●ZHUOQING LI¹, PAI ZHAO¹, PATRICK HUBER², and ROBERT BLICK² — ¹TU Hamburg Institut für Material- und Röntgenphysik, Hamburg, Germany — ²Center for Hybrid Nanostructures, University of Hamburg, Hamburg, Germany

Surface acoustic waves (SAW) are widely used in both industry and science, while liquid crystals are unique fluids exhibiting long-rang order and self-organization. In this work, a combination of SAW and rod-shaped nematic liquid crystals will be studied to explore the tunability of liquid crystal orientations under SAW. Surface acoustic waves are introduced into miniaturized solid-state devices on piezoelectric LiNbO₃ substrates by interlocking metallic gates called interdigitated transduc-

ers (IDT). When a high-frequency sinusoidal signal is applied to the IDT, a mechanical deformation wave will propagate along the surface of the substrate and the induced shear strain will influence the orientation of the nematic liquid crystals on the surface of the substrate. A feature of the nematic phase is that the anisotropic rod-shaped molecules are collectively orientated in preferred directions. Considering the optical anisotropy of rod-shaped liquid crystals, the collective orientation change of liquid crystal molecules under SAW can be analyzed through birefringence measurements. By studying the tunability of the liquid crystal orientation under SAW induced shear component of the wave, we will be able to develop a novel wireless LC-based optical modulator controllable by acoustic stimuli.

MM 23.20 Tue 18:15 P2/OG1+2

Strain-coupled polar textures in ferroelectric nanocylinders — ●SVITLANA KONDOVYCH¹ and IGOR LUKYANCHUK² — ¹Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — ²Laboratory of Condensed Matter Physics, University of Picardie, 80039 Amiens, France

We consider ferroelectric PbTiO₃ nanocylinders of various size hosting strain-coupled polarization vortices. Depending on the cylinder height and radius, the polarization either swirls around the *c*-oriented cylinder axis (*c*-vortex) or falls into the state with the *a*- or *b*-oriented vortex core (*a*-vortex). The emergence of vortices occurs due to the competition of elastic and electrostatic interactions and complies with the Arnold theorem for divergenceless vector fields, which exist as two types of topological excitations, either vortices or Hopfions [2]. In PbTiO₃ cylinders, we observe the geometry- and temperature-induced vortex axis rotation and corresponding transition between the *c*- and *a*-vortex states. The resulting phase diagram, obtained by phase-field modeling in line with analytical calculations, illustrates the variety of polar textures in nanocylinders, applicable for the efficient design of ferroelectric-based device components.

S.K. acknowledges the support from the Alexander von Humboldt Foundation.

[1] S. Kondovych, et al., arXiv:2112.10129v3 (2022).

[2] I. Luk'yanchuk, et al., Nat. Commun. 11, 2433 (2020).

MM 23.21 Tue 18:15 P2/OG1+2

Tuning porous silicon's pore geometry and its influence on laser-excited guided waves — ●MARC THELEN¹, NICOLAS BOCHUD², MANUEL BRINKER¹, CLAIRE PRADA³, and PATRICK HUBER^{1,4,5} — ¹MXP, TUHH, Hamburg, Germany — ²MSME, UPEC, Creteil, France — ³Institut Langevin, ESPCI Paris, Université PSL, CNRS, Paris, France — ⁴CXNS, DESY, Hamburg, Germany — ⁵ChyN, UHH, Hamburg, Germany

Nanoporosity in silicon leads to entirely new functionalities of this mainstream semiconductor with a wide range of applications. In a recent study, we investigated the complex mechanics and the influence of the pores' conicity [1]. This provided the basis for predictable applications in robust on-chip devices and evidence that recent breakthroughs in laser ultrasound technology open up entirely new possibilities for non-destructive in-situ mechanical characterization of dry and liquid-functionalized porous materials. The pores' conicity, which is unintentionally generated during the electrochemical synthesis of porous silicon, can be actively influenced by the process parameters and, within certain limits, arbitrary pore profiles can be generated. This is used, for example, in the production of Bragg mirrors. By tuning the pore shape, we are now investigating its influence on guided waves further, with the goal of developing a phononic material.

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

MM 23.22 Tue 18:15 P2/OG1+2

Unraveling Fluid Phase Behavior in Geometrically Disordered Nanoporous Materials — ●HENRY R. N. B. ENNINFUL and RUSTEM VALIULLIN — Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstraße 5, 04103, Leipzig, Germany.

Mesoporous solids exhibit structural disorder which strongly influence confined fluid properties. This renders quantification of structural disorder and its correlation with physical properties of confined matter a necessary step towards their optimization in practical applications.

In this work, we present advances made in the understanding of correlations between the phase state and geometric disorder in a series of nanoporous solids with variable morphologies. We overview the recently developed statistical theory for phase transitions in a minimalistic model of disordered pore networks represented by the lin-

ear chains of pores with statistical disorder. Furthermore, we show that correlating its predictions with various experimental observations, the model gives notable insights into collective phenomena in phase-transition processes in disordered materials and is capable of explaining self-consistently the majority of the experimental results obtained for gas*liquid and solid*liquid equilibria in mesoporous solids. We also show how a newly-introduced interconnectivity parameter of the pore network can be assessed to describe the morphology of porous solids.

MM 23.23 Tue 18:15 P2/OG1+2

Negative Poisson's Ratio in Hierarchical Nanoporous Gold — ●HAONAN SUN^{1,2}, LUKAS LÜHRS², and SHAN SHI^{1,3} — ¹Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — ²Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — ³Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of crack-free monolithic hierarchical nested network nanoporous gold enables the investigation on the benefits of hierarchy in the aspect of mechanical properties [1]. It has been demonstrated that hierarchical nanoporous gold (HNPG) can achieve a substantially reduced solid fraction and enhanced specific stiffness and strength compared with non-hierarchical nanoporous gold. However, the role of the hierarchical structure on Poisson's ratio is not explored yet. In this work, we synthesize mm-sized HNPG samples out of a Ag₉₃Au₇ master alloy with a dealloying-coarsening-dealloying method. We then explore the elastic and plastic Poisson's ratios of HNPG by using digital image correlation during compression testing. Remarkably, we find Poisson's ratio of HNPG is negative for a given strain regime, which suggests their potential application as auxetic materials. Furthermore, the effect of ligament size at both hierarchy levels on Poisson's ratio is also investigated. [1] S. Shi, Y. Li, B.-N. Ngo-Dinh, J. Markmann and J. Weissmüller, Scaling behavior of stiffness and strength of hierarchical network nanomaterials, Science 371 (6533), 2021.

MM 23.24 Tue 18:15 P2/OG1+2

Mechanical actuation of nanoporous metal driven by electroactive self-assembled monolayers — ●MATTIS OLGA and MAMEKA NADIA — Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous (np) metals fabricated by alloy corrosion are emerging as promising functional materials for (bio-)chemical sensing and actuation. The actuation with np metals exploits the electrocapillary phenomena of metal surfaces, in which surface stress responses to changes of the surface state (e.g. due to adsorption). As the surface stress is coupled with stresses of opposite sign in the metal bulk [1], its variations manifest themselves through macroscopic movements of the entire solid [2].

Due to high surface area, surface-functionalized np metals offer an ideal platform for highly sensitive sensing and actuation technologies. Here, we report reversible electroactuation of unimodal and hierarchical np-Au modified with an electroactive ferrocene-terminated self-assembled monolayer (SAM). In our experiment utilizing in situ dilatometry in electrolyte, an electrode potential is imposed on np-Au modulates redox transformations of SAM by oxidation and reduction of the ferrocene moiety. We find pronounced actuation strain variations that accompany the monolayer structural transformations triggered by potential. We discuss an origin of the phenomena in view of surface stress change of gold surfaces functionalized with the redox-active SAM. [1] Weissmüller, Cahn. Acta Mater. 45(5) 1899 (1997). [2] Kramer, et al. Nano Lett. 4(5) 793 (2004).

MM 23.25 Tue 18:15 P2/OG1+2

Importance of symmetry for the collapse of nanowire arrays — ●MALTE GRÜNERT, CHENGZHANG YANG, HUAPING ZHAO, and YONG LEI — Technische Universität Ilmenau

We present numerical results highlighting the importance of symmetry considerations in the capillary collapse of nanowire arrays. For many of the envisaged applications of nanowire arrays, for example as a novel electrode material in lithium-ion batteries [1], maximizing the aspect ratio of the individual nanowires is one of the main goals. However, collapse occurs for wet-chemical fabrication processes after a critical aspect ratio is exceeded. As the length of the nanowires is increased, the torque resulting from surface tension during the drying step is increased as well, leading to collapse. In literature, only systems consisting of few nanowires are considered [2]. We show using multi-

physics FEM simulations that a perfectly symmetric periodic nanowire array does not collapse, as the forces acting on the nanowires exactly cancel out. However, we also show that even slight length variations below the currently achievable experimental precision suffice to break the symmetry enough to lead to the collapse of the entire array.

[1] L. Liang, Y. Xu, C. Wang, L. Wen, Y. Fang, Y. Mi, M. Zhou, H. Zhao, and Y. Lei, Large-scale highly ordered Sb nanorod array anodes with high capacity and rate capability for sodium-ion batteries, *Energy & Environmental Science*, 8, (2015).

[2] D. Chandra and S. Yang, Stability of high-aspect-ratio micropillar arrays against adhesive and capillary forces, *Accounts of Chemical Research*, 43, (2010)

MM 23.26 Tue 18:15 P2/OG1+2

Architecting Nanoscaffolds to Ward Off Agglomeration of Nanowire arrays: Achieving Reliable Length Retention — ●CHENGZHAN YAN, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany.

Nanowire arrays with well-defined arrangements and high aspect ratios are of particular interest for energy storage systems. To this end, one prevailing strategy is to combine ordered porous templates with wet chemical techniques. However, nanowires with high aspect ratios have a more severe tendency to self-agglomerate because of uneven capillary forces, which leads to poor arrangement reliability and degrades the electrochemical performance. Herein, an ultra-thin honeycomb alumina nanoscaffold (HAN) is constructed to ensure the structural stability of nanowire arrays, achieving a four-fold increase in the aspect ratio over the restriction. Within the integrated architecture, each nickel nanowire is individually separated by HAN so that the capillary forces around the nanowire cancel each other out during drying. Moreover, MnO₂ and polypyrrole are further electrodeposited on these free-standing nanowires to form a vertically aligned core-shell 1D nanostructure arrays as cathodes and anodes for assembling micro-supercapacitors (MSCs). Attributed to the high specific surface area and low charge diffusion resistance, the assembled MSCs attain remarkably improved energy density, rate performance and lifespan.

MM 23.27 Tue 18:15 P2/OG1+2

Porous alumina membranes: how close to perfection? — ●MARINE BOSSERT¹, PANAYOTIS SPATHIS², PIERRE-ÉTIENNE WOLF², LAURENT CAGNON², ISABELLE TRIMAILLE³, and ÉTIENNE ROLLEY⁴ — ¹Institut of Materials Physics and Technology, Hamburg University of Technology, Germany — ²Institut Néel, Grenoble, France — ³Institut des NanoSciences de Paris, Paris, France — ⁴Laboratoire de Physique de l'École Normale Supérieure, Paris, France

Alumina, and to a lesser extent, silicon porous membranes are considered often as model systems made of straight and independent pores, and, as such, porous alumina is used as templates for the synthesis of magnetic or thermoelectric materials [1].

In order to assess to which extent this ideal picture is valid, we have carried out extensive sorption measurements on membranes of different thicknesses, either native or with a pore aperture reduced by Atomic Layer Deposition. For porous silicon membranes, we find constrictions along the pore axis for all samples and interconnections between neighbouring pores when the latter are longer than 2 microns [2]. For alumina membranes, the pores are independent, but conical in shape rather than cylindrical, and rough rather than smooth. Moreover, their average diameter (along their length) is distributed from pore to pore.

We present quantitative estimates of these deviations to ideality, and discuss how to minimize them. [1] Lee and Park *Chemical Reviews* 2014 114 (15), 7487-7556 [2] Bossert et al, *Langmuir* 2021 37 (49), 14419-14428

MM 23.28 Tue 18:15 P2/OG1+2

Freezing of water in 3 nm silica nanopores: A molecular dynamics study — ●LARS DAMMANN^{1,2}, ROBERT HORST MEISSNER^{2,3}, and PATRICK HUBER^{1,2} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany — ²Hamburg University of Technology, Am Schwarzenberg-Campus 1, Hamburg 21073, Germany — ³Institute of Surface Science, Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, Geesthacht 21502, 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

crystallization, the crystalline structures of nanoconfined water and the lower bounds of pore sizes that still permit phase transitions are subject of scientific discussions. Molecular dynamics simulations might support the investigation of open questions about the phase transitions of water in nanoporous systems. However, liquid to solid phase transitions of bulk water are difficult to simulate since the nucleation process is energetically hindered. In strong confinement the phase transition of water is further frustrated which makes a brute force approach computationally unfeasible. Additionally it is difficult to find collective variables for enhanced sampling techniques without knowledge about the target structure. We present our ongoing investigation on if and how MD simulations about the freezing of water in nanoporous media can be conducted with an exemplary silica nanopore structure of 3 nm pore diameter.

MM 23.29 Tue 18:15 P2/OG1+2

Mechanical properties of bicontinuous Ti networks formed via peritectic melting — ●NINA PETERSEN¹, ZHONGYANG LI¹, LUKAS LÜHRS¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg — ²Institute of Materials Mechanics, Helmholtz-Zentrum hereon, Geesthacht

Recent work has shown, that bicontinuous networks can be obtained from TiAg alloys by peritectic melting. These microstructures can then be transformed to open porous networks by selective etching of the Ti or Ag phase. For open porous Ti networks, the ligament size as well as the morphology can be influenced by variation of the melting parameters like temperature and duration of the heat treatment.

In this work, the microstructure of open porous Ti samples was analysed by scanning electron microscopy. The samples were then mechanically tested using continuous compressive loading as well as loading-unloading protocols. The strain was analysed with digital image correlation. The samples exhibit strength values of over 150 MPa that increase with the duration of the heat treatment. This research links the mechanical performance of these Ti networks to the morphological evolution of the microstructures during heat treatment.

MM 23.30 Tue 18:15 P2/OG1+2

Time-resolved EBSD investigation of abnormal grain growth in the aluminum alloy AA5252 — ●KAROLINA HOLÍKOVÁ¹, JULES M. DAKE¹, MADLEN ATZEN¹, THOMAS WILHELM², LUKAS PETRICH², ORKUN FURAT², VOLKER SCHMIDT², BAPTISTE FLIPON³, MARC BERNACKI³, and CARL E. KRILL III¹ — ¹Institute of Functional Nanosystems, Ulm University, Germany — ²Institute of Stochastics, Ulm University, Germany — ³MINES ParisTech, PSL University, France

Heat treatment causes changes in the microstructure of polycrystalline materials, with growth of the average grain size being a prominent example. The driving force is the reduction in free energy of the system. When the average grain size increases monotonically with time but the grain size distribution remains self-similar, the process is called normal grain growth (NGG). In contrast, abnormal grain growth (AGG) is characterized by the much faster growth of a few grains at the expense of neighbors, resulting in a bimodal size distribution. Analytic models and computer simulations do a good job of describing NGG, but they generally fail at predicting AGG in real systems—owing to insufficient knowledge of the underlying mechanism(s). If one could observe sequential microstructural changes during AGG, then one might gain a deeper understanding of the phenomenon. To that end, we have investigated grain growth in the aluminum alloy AA5252, which is known to manifest AGG. Time-resolved electron backscatter diffraction (EBSD) measurements reveal abnormal microstructural evolution in 2D, from which we extract clues regarding the underlying mechanism for AGG.

MM 23.31 Tue 18:15 P2/OG1+2

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

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. Both resistometry and dilatometry are simple online methods to monitor changes in the microstructure of a metallic alloy. In this work we focused on natural and artificial aging of Al-Cu system with samples containing 2 - 4 wt.% of Cu. Natural aging depends on quenched in vacancies, so on the quenching conditions. Samples

were homogenized at various temperatures and rapidly quenched to ambient temperature. Afterwards measurements with both techniques 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 for samples with ternary trace alloying metals than Cu. Dilatometry shows a clear contraction of the samples during GP-zone formation and an expansion, if θ' phase forms.

MM 23.32 Tue 18:15 P2/OG1+2

Circularity: a microstructural clue to the origin of extreme abnormal grain growth in nanocrystalline Pd-Au — ●FABIAN ANDORFER¹, JULES M. DAKE¹, JOHANNES WILD², TORBEN BOLL², DOROTHÉE VINGA SZABÓ², STEFAN WAGNER², ASTRID PUNDT², and CARL E. KRILL III¹ — ¹Institute of Functional Nanosystems, Ulm University — ²Karlsruhe Institute of Technology KIT

Heat treatment causes polycrystalline materials to manifest either normal or abnormal grain growth. During normal growth, the average grain size increases monotonically, but the grain size distribution remains unimodal. In contrast, when abnormal grain growth occurs, some grains acquire a significant growth advantage compared to the remaining matrix grains, resulting in a bimodal distribution of grain sizes. Inert-gas condensed nanocrystalline Pd-Au alloys undergo an extreme form of such abnormal grain growth: While the grain boundaries separating the abnormal and matrix grains in conventional samples tend to be rather smooth, in nanocrystalline Pd-Au the same boundaries take on rough and highly convoluted shapes - similar to a jagged coastline! In such cases, the measurement and calculation of grain circularity has proven to be a promising tool for classifying the nature of a given grain's abnormality. We have determined the circularity of abnormal grains emerging in nanocrystalline Pd-Au samples, and we have compared the results to values reported in the literature or obtained from simulations. From this information, we hope to gain a deeper understanding of the mechanism(s) responsible for the extreme growth mode observed in nanocrystalline Pd-Au.

MM 23.33 Tue 18:15 P2/OG1+2

Manipulating microstructures by means of magnetic fields — ●THOMAS BREDE¹, FERNANDO MACCARI², and RAINER BACKOFEN³ — ¹Institut für Materialphysik, Universität Göttingen, Deutschland — ²Institut für Materialwissenschaften, Technische Universität Darmstadt, Darmstadt — ³Institut für wissenschaftliches Rechnen, Technische Universität Dresden, Dresden

In this project, the isolated influence of strong magnetic fields on the development of the microstructure of ferromagnetic thin films during annealing processes is investigated. For this purpose, thin films out of Iron, Nickel and Cobalt are prepared and characterized, then heat treated in the same heater with and without magnetic field and subsequently characterized. The experiments are accompanied by phase field crystal modeling to separate the different possible influences on the microstructure.

Through the parallel approach of experimental and modeling work, the effect of external magnetic fields on the development of microstructure and grain orientation will be investigated to understand the direct effect of the magnetic field. Through a deeper understanding of the isolated influence of a magnetic field, additional conclusions should be

possible about the influence of induced magnetic fields in the case of sample treatment with high currents.

MM 23.34 Tue 18:15 P2/OG1+2

Anharmonicity of the antiferrodistortive soft mode in barium zirconate BaZrO₃ — ●PETER ROSANDER¹, ERIK FRANSSON¹, COSME MILESI-BRAULT^{2,3,4}, CONSTANCE TOULOUSE², FRÉDÉRIC BOURDAROT⁵, ANDREA PIOVANO⁵, ALEXEI BOSSAK⁶, MAEL GUENNOU², and GÖRAN WAHNSTRÖM¹ — ¹Chalmers University of Technology, Göteborg, Sweden — ²University of Luxembourg, Belvaux, Luxembourg — ³Luxembourg Institute of Science and Technology, Belvaux, Luxembourg — ⁴Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — ⁵Institut Laue-Langevin, Grenoble, France — ⁶European Synchrotron Radiation Facility, Grenoble, France

Few perovskites adopt the ideal cubic phase at low temperatures. However, a promising candidate to, on average, remain cubic, even at 0K, is barium zirconate. The competing phase is a structure with sequentially tilted oxygen octahedra. This distortion is driven by the soft tilt mode at the R-point of the cubic Brillouin zone.

We report data from inelastic neutron scattering (INS) on a single crystal of barium zirconate. This reveals that the tilt mode softens substantially from 9.4 meV at room temperature to 5.6 meV at 2K. Additionally, the INS measurement unveils that the acoustic phonon mode at the same point in the Brillouin zone is almost temperature independent, which is in stark contrast to the tilt mode. The theoretical calculations show that it is critical to account for quantum fluctuations in order to correctly reproduce the experimental temperature dependence.

MM 23.35 Tue 18:15 P2/OG1+2

Terahertz third harmonic generation from a correlated metal — ●GULLOO LAL PRAJAPATI¹, SERGEY KOVALEV¹, JAN-CHRISTOPH DEINERT¹, ALEXEY PONOMARYOV¹, ATIQA ARSHAD¹, GAURAV DUBEY², and DHANVIR SINGH RANA² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal, India

High harmonic generation, a result of intense nonlinear light-matter interaction, has exciting prospects for probing fundamental ultrafast dynamics in matter and it is the basis for attosecond photonics [1, 2]. Here, we present an experimental study on terahertz (THz) third harmonic generation (THG) on a correlated metal, LaNiO₃ which exhibits non-Fermi liquid type of metallic state [3]. We observe an intense THG signal, which is usually not expected in metals, upon pumping it by 0.3 THz pulses with peak fields of about 100 kV/cm. Decreasing temperature or increasing fluence increases the intensity of this THG signal. We speculate the origin of such THG emission could be due to the anharmonic nature of LaNiO₃ conduction band caused by electronic correlation or directional nature of Ni-3d orbitals. Further investigations are under way to pinpoint the exact mechanism of the observed THG. Our study paves the way for THz THG emission from strongly correlated systems, and enables tracking of their properties on ultrafast timescales. References: 1. Nature Photon 12, 266, 270 (2018). 2. Nature 561, 507, 511 (2018). 3. Annu. Rev. Mater. Res. 46, 305-34 (2016).

MM 24: Invited Talk: Barnoush

Time: Wednesday 9:30–10:00

Location: SCH A 251

Invited Talk

MM 24.1 Wed 9:30 SCH A 251

Characterization of hydrogen effect on mechanical properties of metals at different length scales — ●AFROOZ BARNOUSH, PRINCE BARANWAL, and HANAN FARHAT — Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), P.O. Box 34110, Doha, Qatar

Conventional macroscopic mechanical tests cannot resolve the spatiotemporally distributed hydrogen interaction with the metal microstructure under stress and give us enough information to develop

predictive models for the hydrogen effect on mechanical properties. They typically measure an integration of these incidents over time, which manifests in loss of ductility, hence hydrogen embrittlement. Therefore, it is necessary to isolate these incidents and study them separately. To realize it, we develop mechanical testing approaches at different length scales to look at the interaction of hydrogen with different types of defects and how they behave in the presence of hydrogen. This talk will give an overview of the work that has been done in the past 20 years to get an insight into the hydrogen effect on mechanical properties at different length scales.

MM 25: Development of Computational Methods: Crystal Structure and Properties

Time: Wednesday 10:15–11:30

Location: SCH A 251

MM 25.1 Wed 10:15 SCH A 251

A hybrid multiscale phase-field crystal, amplitude phase-field crystal approach - elastic properties and numerical studies — ●MAIK PUNKE and MARCO SALVALAGLIO — Technische Universität Dresden, Institut für Wissenschaftliches Rechnen, Bürogebäude Z21, Zellescher Weg 25, 01217 Dresden

The modeling of crystalline materials requires the resolution of microscopic details on large length and time scales to guarantee the description of lattice-dependent features as well as the dynamics of solidification. The so-called phase-field crystal (PFC) model emerged as a prominent framework to model crystalline systems. Indeed, it describes crystalline materials through a continuous order parameter related to the atomic number density and its dynamic at relatively large (diffusive) time scales. The amplitude expansion of the PFC model (APFC) was developed to further overcome the length scale limitations in the PFC framework. Herein, the continuous density in PFC models is replaced by the amplitudes of the minimum set of Fourier modes (wave vectors) for a given crystal symmetry.

We propose a multiscale model with local PFC accuracy and APFC length scale limitations. In our hybrid multiscale approach, the PFC and APFC models are coupled through Dirichlet conditions by penalty terms within the spectral framework. We showcase the model capabilities via selected numerical investigations which focus on the energetic and elastic properties of two-dimensional crystals. Furthermore, runtime and accuracy comparisons with the standard PFC and APFC models are made.

MM 25.2 Wed 10:30 SCH A 251

Corrosion evolution in Mg-based alloys: the role of precipitates studied by synchrotron X-ray nanotomography — ●TATIANA AKHMETSHINA¹, ROBIN E. SCHÄUBLIN¹, ANDREA M. RICH¹, NICHOLAS W. PHILLIPS², and JÖRG F. LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — ²Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

Magnesium alloys are very promising candidates for light-weight and bioresorbable medical applications. However, being an active metal, magnesium is susceptible to localized corrosion caused by precipitates or solute elements. In this work, we compare the corrosion behaviour of lean Mg-Ca (X0), developed in our laboratory, with the well-known Mg-Y-Nd-Zr (WE43) alloy that is currently deployed as biomedical material. X0 alloys (0.2-0.6 wt.% Ca) offer a combination of high strength and high ductility and can be considered a safe substitute for WE43 in bioresorbable implants. Using the 3D ptychography technique at the cSAXS beamline of the Swiss Light Source, we monitored the corrosion evolution in X0 and WE43. Both exhibit very different precipitates, which can be distinguished by their electron density in X-ray imaging. We found that the rare-earth-rich precipitates in WE43 tend to remain in the corrosion layer, whereas the Ca-rich ones in X0 predominantly dissolve without any pitting effect. The appearance of the corrosion product and the related chemical composition were also quite different. These findings of in-vitro corrosion can help to better understand the in-vivo degradation of Mg-based biomedical devices.

MM 25.3 Wed 10:45 SCH A 251

Amplitude expansion of the phase-field crystal model for complex crystal structures — ●MARCELLO DE DONNO¹ and MARCO SALVALAGLIO^{1,2} — ¹Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — ²Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

The phase field crystal model allows for studying phenomena on atomic length and diffusive time scales. It accounts for elastic and plastic deformation in crystals, including several processes such as crystal growth, dislocation dynamics, and microstructure evolution. The amplitude expansion of the phase field crystal model describes the atomic density by a small set of slowly-oscillating Fourier modes, making it possible to tackle large three-dimensional systems. However, only basic crystal symmetries have been studied so far. We present a general treatment of virtually any lattice symmetry using the amplitude phase field crystal model, incorporating approaches originally proposed for the phase field crystal model which enable the treatment of non-trivial lattices. We discuss the stability of selected crystal structures, focusing on non-Bravais lattices. As pivotal examples, we show that the proposed approach allows a coarse-grained description of the kagome lattice, exotic square arrangements, and the diamond lattice, hosting dislocations.

MM 25.4 Wed 11:00 SCH A 251

Efficient molecular dynamics simulations using fourth-generation neural network potentials — ●EMIR KOCER^{1,2}, ANDREAS SINGRABER³, Tsz Wai Ko^{1,2}, JONAS FINKLER⁴, PHILIPP MISOF³, CHRISTOPH DELLAGO³, and JÖRG BEHLER^{1,2} — ¹Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, Bochum, Germany — ²Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Bochum, Germany — ³Institut für Experimentalphysik, Universität Wien, Wien, Austria — ⁴Departement Physik, Universität Basel, Basel, Switzerland

Machine learning potentials (MLP) have become a common tool in materials modelling due to their ability to bridge the gap between ab initio and classical molecular dynamics. A limitation of most MLPs, however, is the locality approximation in that only interactions within a cutoff range are considered. This could lead to inaccurate dynamics in systems with relevant long-range interactions. Recently, a fourth-generation of MLPs has 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. In this study, a modified version of 4G-HDNNPs with enhanced efficiency will be presented. The new algorithm has been implemented in the LAMMPS software and tested in large-scale molecular dynamics simulations.

MM 25.5 Wed 11:15 SCH A 251

Sampling-free determination of accurate free energies: A bond lattice mean-field model for central potentials — ●RAYNOL DSOUZA¹, THOMAS SWINBURNE², LIAM HUBER³, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — ²CINaM, Campus de Luminy, 13288 Marseille, France — ³Grey Haven Solutions, Victoria, Canada

The computation of accurate anharmonic free energies at finite tem-

peratures commonly involves the sampling of a large number of configurations. The commonly used (quasi)-harmonic approximation sacrifices physical fidelity by only sampling very few of these configurations. A recent study by the co-authors showed that a mean-field of a lattice of uncorrelated anharmonic first nearest-neighbour bonds can be used to approximate anharmonic free energies of fcc crystals with meV/atom accuracy when paired with a polarized bonding potential [1], thus recapturing an approximation of the anharmonic contributions with minimal computational expense. We extend this approach

to central potentials, while maintaining the original constraints of material compatibility and thermodynamic self-consistency of the model. Using a parameterized bonding potential generated from a few T=0 K ab initio calculations [2] for fcc aluminium, we show that the model yields free energies close to meV/atom of those calculated from ab initio thermodynamic integration for a fraction of the computational effort. [1] Swinburne et al., Phys. Rev. B 102, 100101(R) (2020) [2] Glensk et al., Phys. Rev. Lett. 114, 195901 (2015)

MM 26: Interface Controlled Properties and Nanomaterials: Grain Boundaries and Stability, Spectroscopy and Interatomic Potentials

Time: Wednesday 10:15–13:00

Location: SCH A 216

MM 26.1 Wed 10:15 SCH A 216

Grain-boundary segregation effects on bicrystal Cu pillar compression — •TOBIAS BRINK, MOHAMMED KAMRAN BHAT, JAMES BEST, and GERHARD DEHM — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

It is well known that segregation to grain boundaries (GBs) can modify the mechanical properties of metals, leading for example to improved strength, but also to detrimental effects like embrittlement. Despite this, the nanoscale mechanisms of these changes are currently not fully understood. Here, we present the results of atomistic computer simulations of bicrystalline Cu pillar compression and corresponding micromechanics experiments. The experiments show that Ag segregation to the GB increases the yield stress of the pillars, but only slip traces observed post mortem hint towards the mechanisms. We prepared segregated GB structures with combined molecular dynamics/Monte-Carlo simulations by matching the resulting excess Ag concentration to atom probe tomography results. The virtual nanopillars were cut from this material and varying amounts of dislocation loops were inserted in order to model the pre-existing dislocation networks in the experiment. Switching the atomic types of the segregants between Ag and Cu allowed us to model the exact same pillar and dislocation network with and without segregation, thereby enabling an investigation of the mechanisms underlying the experimentally observed strengthening.

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).

MM 26.2 Wed 10:30 SCH A 216

When grains go wild! Tracing microstructural outcomes back to possible mechanisms for abnormal grain growth — •CARL E. KRILL III¹, ELIZABETH A. HOLM², JULES M. DAKE¹, RYAN COHN², KAROLÍNA HOLÍKOVÁ¹, and FABIAN ANDORFER¹ — ¹Ulm University, Ulm, Germany — ²Carnegie Mellon University, Pittsburgh, PA, USA

Usually, the coarsening of a polycrystalline material is a civilized affair, with adjacent grains swiping atoms so surreptitiously that relative growth rates remain moderate, and the mutual boundary stays smooth. In some cases, however, certain participants in this competition give free rein to an innate hunger for growth! The result is a subpopulation of large, “abnormal” crystallites embedded in a matrix of much smaller grains, whereby the abnormal/matrix interface can be anywhere from perfectly flat to fractally convoluted. The formation of such a microstructure is the telltale signature of abnormal grain growth (AGG). Although the most prominent feature of AGG is the shape of the abnormal grains, simulations indicate that the mechanism of AGG is encoded to a greater extent in the morphology of the interfaces between abnormal and matrix grains. Based on this finding, we propose a scheme for inferring the possible mechanism(s) underlying any experimentally observed case of (sufficiently extreme) AGG, and we illustrate our phenomenological method with experimental examples taken from the literature. Surprisingly, in the most clear-cut cases of AGG we have encountered, microstructural outcomes point to boundary-to-boundary mobility variation as the sole governing factor.

MM 26.3 Wed 10:45 SCH A 216

Influence of precipitates during anodization of aluminum alloys studied by TEM at cryogenic temperatures — •LYDIA DAUM, STEFAN OSTENDORP, MARTIN PETERLECHNER, and GERHARD WILDE — Westfälische-Wilhelms-Universität, Münster, Germany

Aluminum alloys with predefined alloying elements are chosen regarding their performance in certain areas of industrial applications due to their hardness, strength and corrosion resistance. Precipitates such as Mg₂Si and dispersoids, e.g. enrichments of Mn in EN * AW6xxx alloys hinders the formation of ordered anodic aluminum oxides (AAOs) as achievable using high-purity aluminum samples.

The focus of this work is on correlating the structural and chemical properties of precipitates within AAOs and at the interface to the alloy. Due to geometry and size of the precipitates, transmission electron microscopy (TEM) is performed at selected areas. Measuring the same properties inside an Al 6xxx alloy close to the interface provides information about the contribution of the segregations during anodization. Previous scanning transmission electron microscopy (STEM) studies have shown that cryogenic temperatures can partially reduce the beam damage in electron beam sensitive materials as organics or AAOs [1]. In this study, the sample is also characterized by nanobeam diffraction pattern analysis and electron dispersive X-ray spectroscopy at cryogenic temperatures.

[1] A. M. Jasim, X. He, Y. Xing, T. A. White, and M. J. Young. ACS Omega 6.13 (2021), 8986-9000.

MM 26.4 Wed 11:00 SCH A 216

Disconnection-mediated migration of interfaces: continuum modeling and applications — •MARCO SALVALAGLIO¹, CAIHAO QUI², JIAN HAN², and DAVID J. SROLOVITZ³ — ¹Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — ²Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR, China — ³Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China

We present a model for the motion of arbitrarily curved interfaces that respects the underlying crystallography of two phases/domains meeting at an interface and is consistent with microscopic mechanisms of interface motion, i.e., migration of disconnection (line defects in the interface with step and dislocation character) [1]. The equation of motion for interface migration under the influence of a wide range of driving forces is discussed with the aid of numerical simulations [1,2]. A diffuse interface framework is also used to handle complex morphology and deliver proof of concept for microstructure evolution [2]. Recent results achieved with this model, concerning grain boundary morphologies, the competition among thermodynamic and kinetic effects, and grain rotation will be illustrated. [1] J. Han et al. Acta Materialia 227, 117178, (2022). [2] M. Salvalaglio et al. Acta Materialia 227, 117463, (2022).

MM 26.5 Wed 11:15 SCH A 216

Simulated mechanical deformations 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 indenter. 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.

15 min. break

MM 26.6 Wed 11:45 SCH A 216

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

Binary alloys of silver and palladium have recently attracted attention due to their importance in catalysis and nanotechnology. However, the binary Ag-Pd system lacks reliable and efficient interatomic potentials that provide an accurate description of structural and thermodynamic properties, in particular for atomistic simulations of nanoparticles. In this work, we present an atomic cluster expansion (ACE) parametrized for binary Ag-Pd. We show that the Ag-Pd ACE potential provides an ab-initio accurate description of elastic, structural and thermodynamic properties of both, elements as well as their compounds. We demonstrate the computational efficiency and the applicability of our ACE for atomistic investigations of complex phenomena in Ag-Pd nanoparticles.

MM 26.7 Wed 12:00 SCH A 216

Spin-orbit interactions in plasmonic crystals probed by site-selective cathodoluminescence spectroscopy — MASOUD TALEB¹, ●MOHSEN SAMADI¹, FATEMEH DAVOODI¹, MAXIMILIAN BLACK¹, JANEK BUHL², HANNES LÜDER², MARTINA GERKEN², and NAHID TALEBI^{1,3} — ¹Institute of Experimental and Applied Physics, Kiel University, Germany — ²Integrated Systems and Photonics, Faculty of Engineering, Kiel University, Germany — ³Kiel, Nano, Surface, and Interface Science, Kiel University, Germany

The study of spin-orbit coupling (SOC) of light is crucial to explore the light-matter interactions in sub-wavelength nanostructures with broken symmetries. Herein, we explore the SOC in a plasmonic crystal, both theoretically and experimentally. Cathodoluminescence (CL) spectroscopy combined with the numerically calculated photonic band structure reveals an energy band splitting that is ascribed to the behavior of light in the plasmonic crystal where the inversion symmetry is locally broken. By shifting the impact position of the electron beam throughout a unit cell of the plasmonic crystal, we show that the emergence of the energy band splitting strongly depends on the excitation position of the surface plasmon (SP) waves on the crystal. Moreover, we exploit angle-resolved CL and dark-field polarimetry to demonstrate polarization-dependent scattering of SP waves interacting with the plasmonic crystal. Our study gives insight into the design of novel plasmonic devices with polarization-dependent directionality of the Bloch plasmons.

MM 26.8 Wed 12:15 SCH A 216

Soft and Hard X-ray Circular Dichroism in Valence-Band and Core-Level Momentum Microscopy — ●O. TKACH^{1,2}, O. FEDCHENKO¹, K. MEDJANIK¹, Y. LYTVYENENKO¹, S. BABENKOV¹, D. VASILYEV¹, Q.L. NGUYEN³, T.P. VO⁴, T.R.F. PEIXOTO⁵, A. GLOSKOVSKI⁵, C. SCHLUETER⁵, M. HOESCH⁵, D. KUTNYAKHOV⁵, M. SCHOLZ⁵, L. WENTHAUS⁵, N. WIND^{5,6}, S. MAROTZKE⁵, A. WINKELMANN⁷, J. MINAR⁴, K. ROSSNAGEL^{5,8}, H.-J. ELMERS¹, and G. SCHÖNHENSE¹ — ¹Univ. Mainz — ²SSU, Ukraine — ³SLAC Nat. Accel. Lab., USA — ⁴Univ. West Bohemia, Czech — ⁵DESY Hamburg — ⁶Univ. Hamburg — ⁷AGH Univ., Poland — ⁸Univ. Kiel

We introduce full-field mapping of the circular dichroism texture in X-ray momentum microscopy. I(EB,k) energy-momentum space tomography with both soft and hard X-rays at PETRA-III yields CDAD patterns. Kinetic energies of up to >7 keV and a large k-field-of-view enable capturing of structural information via XPD Kikuchi patterns, which show pronounced asymmetries. Patterns at different azimuthal angles exhibit sharp zero lines, when the helicity vector lies in a mirror plane. Similar zero lines also appear in the XPD patterns of core levels, as exemplified for Ge 3p, Si 2p and various W core levels at $h\nu = 6$ keV. Calculations using Bloch-wave approach and one-step photoemission show good agreement with experiment. In order to disentangle the contributions of the photoexcitation (intrinsic part) from the Kikuchi process (extrinsic), XPD has been implemented in the Munich SPRKKR package, unifying one-step model of photoemission and multiple scattering theory.

MM 26.9 Wed 12:30 SCH A 216

Direct writing of three-dimensional nano-superconductors — ●ELINA ZHAKINA¹, MARKUS KÖNIG¹, SEBASTIAN SEIFERT¹, AMALIO FERNÁNDEZ-PACHECO², PAUL SIMON¹, WILDER CARRILLO-CABRERA¹, and CLAIRE DONNELLY¹ — ¹Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — ²Institute of Nanoscience & Materials of Aragón CSIC-University of Zaragoza, Zaragoza, Spain

In recent years, superconductivity and vortex matter in curved 3D nanoarchitectures have become a vibrant research avenue because of the rich physics of the emerging geometry- and topology-induced phenomena [1]. However, the fabrication of such architectures is still challenging. Currently, fabrication techniques of innovative three-dimensional (3D) nano-objects are being developed [2].

Here, we present a new route to fabricating superconducting 3D nanoarchitectures by focused electron-beam-induced-deposition [3] of tungsten, allowing for the realisation of complex 3D superconducting geometries with a critical temperature on the order of 5 K. We observe a geometrical effect of the 3D nanoarchitecture, namely, the angular dependence of the upper-critical magnetic field that is not possible in bulk superconductors. This method unveils a wide perspective in experimental studies of the dynamics of topological defects in curved 3D nanoarchitectures.

[1] V. M. Fomin et al, Appl. Phys. Lett. 120, (2022) [2] R. Corboda et al, Beilstein J. Nanotechnol, 11, (2020) [3] L. Skoric et al, Nano Letters 20 (2020)

MM 26.10 Wed 12:45 SCH A 216

Influence of a p-n Heterojunction on the Diffusive Transport in Tungsten Trioxide Thin Films — ●JAN L. DORSEIFER^{1,2}, MARKUS S. FRIEDRICH^{1,2}, and PETER J. KLAR^{1,2} — ¹Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — ²Center for Materials Research (ZfM), Justus-Liebig-University, Giessen, Germany

Tungsten trioxide (WO₃) is (typically) an n-type semiconductor and a prominent electrochromic material. It changes its optical properties when charge carriers are inserted. Due to its excellent electrochromic properties, WO₃ is the most commonly used functional material in so called "smart" windows which are a promising technology for significantly lowering the energy consumption for building climatization. Industrially manufactured polycrystalline WO₃ thin films were coated with p-type nickel monoxide (NiO_x) thin films by ion beam sputter deposition. In order to investigate the diffusive transport of hydrogen in WO₃ thin films influenced by a p-n heterojunction, spatially and temporally resolved optical transmission measurements are conducted on NiO_x/WO₃-heterostructures during the potentiostatic coloration of the WO₃ thin films. Spatial and temporal diffusion profiles determined by analyzing these measurements indicate that the lateral propagation of hydrogen in NiO_x coated WO₃ films is accelerated. In addition, an increased transmittance is observed in the colored state. To describe these findings, a model is set up based on an increase in hydrogen concentration inside the WO₃ layer outside the space-charge region formed at the NiO_x/WO₃ interface.

MM 27: Hydrogen in Materials

Time: Wednesday 10:15–13:00

Location: SCH A 215

MM 27.1 Wed 10:15 SCH A 215

Strain-induced twins and martensite: Effects on hydrogen embrittlement of additive manufactured (AM) 316L

— ●STEFAN WAGNER¹, YUANJIAN HONG², CHENGSHUANG ZHOU², SABINE SCHLABACH^{1,3}, ASTRID PUNDT¹, LIN ZHANG⁴, and JINYANG ZHENG⁴ — ¹Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — ²Institute of Material Forming and Control Engineering, Zhejiang University of Technology, Hangzhou, China — ³Karlsruhe Nano Micro Facility (KNMF), KIT-Campus North, Eggenstein-Leopoldshafen, Germany — ⁴Institute of Process Equipment, Zhejiang University, Hangzhou, China

Extending the use of hydrogen as a renewable energy carrier 316L is one of the most important structural materials. Additive manufacturing significantly enhances the steels' strength, allowing for weight reduction of construction parts. In this contribution [1] we investigate effects of strain-induced twins and martensite on hydrogen embrittlement of AM316L under tension in the temperature range from 80 K to 300 K. It is revealed that quasi-cleavage of twin boundaries is the major path of material failure. Strain-induced martensite has low impact on the H-embrittlement of AM316L, since it emerges only late in the deformation process.

[1]: Yuanjian Hong et al., 2022. Corrosion Science, 208; 110669-1-16.

MM 27.2 Wed 10:30 SCH A 215

Ab-initio insights into hydrogen-carbide interaction in bcc Fe

— SAURABH SAGAR and ●POULUMI DEY — Delft University of Technology, Delft, The Netherlands

Development of advanced high-strength steels is in high demand owing to its wide scale applications. The excellent mechanical properties of these steel grades are attributed to the underlying microstructure which comprises of finely dispersed nano-precipitates. However, one major factor restricting their application is their susceptibility to Hydrogen Embrittlement (HE). Experimental and theoretical work have been carried out to understand if the nano-sized carbides can aid in reducing the susceptibility to HE along with providing strengthening. Within this study, we investigated the effectiveness of finely dispersed nano-carbides (i.e., TiC, NbC and VC) to limit the diffusible hydrogen content in bcc Fe. Our study revealed that the interplay between hydrogen and carbon vacancies, local atomic environment at interface as well as interface geometry can lead to significantly increased hydrogen solubilities. Thus, the trapping at these sites leads to a reduction in concentration of diffusible hydrogen. However, the question remains whether hydrogen can populate the deepest traps (i.e., the carbon vacancies) in the bulk of these carbides. We, thus, extended our study to compute migration barriers of hydrogen across the coherent interface between bcc Fe and TiC, NbC and VC using climbing-image Nudged Elastic Band method. Furthermore, we evaluated whether a chain of interconnected carbon vacancies from the interface to the bulk of the carbides leads to a reduction in the migration barrier of hydrogen.

MM 27.3 Wed 10:45 SCH A 215

Role of diffusible hydrogen on the mechanical behavior of bcc alloys by in situ micromechanics during hydrogen charging —

●MARIA JAZMIN DUARTE CORREA, JING RAO, and GERHARD DEHM — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Hydrogen embrittlement represents a major challenge for the use of hydrogen (H) as energy carrier. Understanding individual hydrogen-microstructure interactions by targeting analyses at the nano-/microscale during H exposure is essential to prevent material degradation. We will present nanoindentation and micropillar compression tests during H charging of Fe-Cr alloys (8-20 wt.%Cr) using our novel "back-side" electrochemical H charging approach for nanoindentation related techniques. 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 as well analyzed in terms of the diffusion behavior and used to develop a nanohardness-based H diffusion coefficient approach. On the other hand, 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 which will be shown

using the example of the model alloys mentioned above.

MM 27.4 Wed 11:00 SCH A 215

Hydrogen interstitials in iron oxides using ab-initio calculations —

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

The steel making industry is responsible for more than 6% of CO₂ emissions. These emissions come from the dependency on carbon and carbon monoxide as reducing agents. Hydrogen, on the other hand, can reduce iron oxides with water released instead. The reduction route from Magnetite to Hematite, then Wüstite, and finally to pure iron requires hydrogen to diffuse into and react with the different solid structures as well as with the multiple solid-solid interfaces. To optimize the reduction process, the mechanistic details of this process requires understanding to the role of hydrogen interstitials in the bulk iron oxides. We therefore computed the diffusion paths of hydrogen through the different iron oxide phases employing density functional theory (DFT) calculations for all three iron oxides - Magnetite, Hematite, and Wüstite. Analyzing the electronic structure of the studied oxides, we examine the reliability of the used exchange correlation functionals and how the electronic structure is affected by the inclusion of hydrogen, both as a neutral and a charged point defect. Finally, we utilize symmetrized plane waves to map the full 3D potential energy surfaces (PESs) for hydrogen interstitials within these iron oxides using a modest number of DFT calculations. Based on these calculations we identify the hydrogen preferential interstitial sites, diffusion barriers, and diffusion paths.

MM 27.5 Wed 11:15 SCH A 215

Influence of impurity atoms on the hydrogen diffusion into ruthenium —

●JULIAN GEBHARDT and DANIEL URBAN — Fraunhofer IWM, 79108 Freiburg

Ruthenium is considered as a promising protection layer to prevent the penetration of small atoms such as hydrogen into the underlying material. However, hydrogen is known to be able to penetrate ruthenium films under certain conditions and it has been hypothesized that impurity atoms, such as Sn, could play a major role in this process, decreasing the barrier of diffusion into the material for incoming hydrogen. We demonstrate that this is not the case for low to medium coverages, i.e., as long as the adsorbed species can be treated individually without significant adsorbate-adsorbate interactions. Within this coverage regime, the hydrogenation is destabilized in the vicinity of impurity atoms, such as X=Mg, P, S, Si, or Zn, due to the strong bonding of the adsorbates with the free ruthenium surface. As a result, the diffusion barriers are not significantly reduced in the vicinity of any of the tested impurity atoms. The most likely and energetically favorable process occurs at a sufficiently large distance to the impurity, with an energy barrier that is almost identical to that of the free surface. Due to the chemical variety of the considered impurity atoms, this finding appears to be general. This means that impurities can be ruled out to enhance hydrogen uptake of ruthenium layers for the considered coverages and other structural properties such as grain boundaries and dislocations should be considered as pathway for the hydrogen penetration.

15 min. break

MM 27.6 Wed 11:45 SCH A 215

Metal Hydride Materials for Solid-State Hydrogen Storage Applications: Utilizing the Synergy of Experiment & Theory for Future Materials Design Challenges —

PAUL JERABEK¹, ●BRANDON WOOD², TAE WOOK HEO², and CLAUDIO PISTIDDA¹ — ¹Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — ²Materials Science Division, Lawrence Livermore National Laboratory (LLNL), Livermore, USA

Metal hydride materials present a safe, efficient and long-term storage option for hydrogen under mild conditions for many stationary and mobile applications and will play an important role in the transition towards an emission-free energy economy.

Deep understanding of (de)hydrogenation thermodynamics and kinetics of such materials is essential to enable targeted design of novel

storage materials and optimization of existing compositions tailored for specific applications. To obtain the necessary insights, computation and experiment need to work closely together to fully leverage theory-experiment feedback loops.

In this talk, an overview will be given of how experimental activities can be connected with computational multi-scale methodology (from atomistic to mesoscale), as currently performed in the joint efforts by the metal hydride materials research groups at Hereon and LLNL, with the goal being to develop virtual workflows linking Density Functional Theory methods, thermodynamic modeling and phase-field simulations together with experimental investigations for an integrated description of metal hydride (de)hydrogenation processes.

MM 27.7 Wed 12:00 SCH A 215

Ab Initio Simulations of Laves-phase high-entropy alloys for hydrogen storage — ●YUJI IKEDA¹, KAVEH EDALATI², and BLAZEJ GRABOWSKI¹ — ¹University of Stuttgart, Stuttgart, Germany — ²Kyushu University, Fukuoka, Japan

High-entropy alloys (HEAs), particularly those in the Laves phases, are promising candidates for hydrogen-storage alloys. Recent experiments have indeed revealed that the equiatomic TiZrCrMnFeNi Laves-phase HEA can work as a hydrogen-storage alloy at room temperature (i.e., without heating) under nearly atmospheric pressure [1,2]. Tuning the compositions of such Laves-phase HEAs should be possible to design hydrogen-storage alloys with more desirable properties. We have demonstrated that ab initio H adsorption energies in $Ti_xZr_{2-x}CrMnFeNi$ become more negative (thus energetically more favorable) on average with increasing the Ti content, consistent with experiments [3]. We will also show how the H adsorption energy depends on the local chemical environment in the Laves-phase HEAs.

[1] P. Edalati, A. Mohammadi, Y. Li, H.-W. Li, R. Floriano, M. Fuji, and K. Edalati, *Scr. Mater.* 209, 114387 (2022).

[2] P. Edalati, R. Floriano, A. Mohammadi, Y. Li, G. Zepon, H.-W. Li, and K. Edalati, *Scr. Mater.* 178, 387 (2020).

[3] A. Mohammadi, Y. Ikeda, P. Edalati, M. Mito, B. Grabowski, H.-W. Li, and K. Edalati, *Acta Mater.* 236, 118117 (2022).

MM 27.8 Wed 12:15 SCH A 215

Visualizing radiation-induced damage by Hydrogen/Deuterium — ●APARNA SAKSENA, BINHAN SUN, HEENA KHANCHANDANI, and BAPTISTE GAULT — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf 40237, Germany

Atom probe tomography (APT) is now extensively used to measure the local chemistry of materials. APT proceeds by field evaporating a sharp, needle-shaped specimen with a radius ~ 50 nm, often prepared by focused ion beam (FIB) milling. The interaction of the ion beam at high currents is known to amorphize crystalline materials by changing the lattice and creating vacancies. Therefore, a platinum protective layer and a low-energy ion shower are routinely used to avoid or remove the damaged layer from the specimen. Additionally, for investigating the local chemistry of defects such as interfaces via APT, transmission Kikuchi diffraction (TKD) can be performed during milling steps. The damage resulting from these techniques is considered negligible. Here, we use deuterium charging to probe the

damage associated with specimen preparation as vacancies are known to be strong trapping sites for hydrogen/deuterium. We analyzed a medium Mn steel containing austenite (fcc) and ferrite (bcc). APT specimens were charged in a deuterium gas atmosphere, and the distribution of deuterium shows clusters of point defects after Pt deposition, conventional Ga-FIB preparation, and TKD. These deuterium-rich clusters are sequentially minimized by systematically eliminating these preparation-induced damages.

MM 27.9 Wed 12:30 SCH A 215

Mechanism-based Lifetime Assessment under the Influence of Hydrogen — ●FABIEN EBLING^{1,2}, HEINER OESTERLIN², ASTRID PUNDT¹, and KEN WACKERMANN² — ¹Karlsruhe Institute of Technology (KIT) Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — ²Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Components see a variety of mechanical and thermal loads during service. Increased damage can occur when used in a hydrogen atmosphere. The experimental investigation of all states is very time-consuming and expensive, especially for testing under hydrogen influence. Mechanism-based lifetime assessments can be used to model crack growth and predict service life. This can significantly reduce the need of experimental investigations for a safe design of components. This work discusses different approaches of modeling hydrogen assisted cracking and presents an adaptation of the ZD parameter according to Heitmann (1983) for the influence of hydrogen at different temperatures.

MM 27.10 Wed 12:45 SCH A 215

Validation of continuum simulations of materials at the mesoscopic level with X-ray and neutron diffraction with a focus on hydrogen storage materials — ●ARNAB MAJUMDAR¹, MARTIN MÜLLER², and SEBASTIAN BUSCH¹ — ¹GEMS at MLZ, Helmholtz-Zentrum hereon GmbH, Lichtenbergstr. 1, 85748 Garching, Germany — ²Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH, Max-Planck-Str. 1, 21502 Geesthacht, Germany

With the advent of new technologies, it has been possible to design new materials through theoretical analysis and simulation. However, these simulations have to be validated by experiments. In this work, we develop a method to validate the structural features in continuum simulations directly on the mesoscopic level with X-ray and neutron scattering experiments. The workflow to compare atomistic computer simulations to scattering patterns is well established: the scattering amplitude of individual atoms is summed, whose positions are obtained from the simulation. This approach fails for larger mesoscopic structures due to the unrealistic computation time required to generate the simulations and scattering pattern on a mesoscopic scale with atomic resolution. We developed a methodology that calculates scattering patterns from a continuum simulation like phase-field modeling, where the material description is continuous instead of a collection of atoms. The approach is validated with simple structures and gradually applied to more complex structures. The long term goal is to use this technique for the simulation of hydrogen storage materials and validation of the simulations with scattering data.

MM 28: Liquid and Amorphous Metals

Time: Wednesday 10:15–12:45

Location: SCH A 118

MM 28.1 Wed 10:15 SCH A 118

Relation between decoupled α and β relaxation processes and medium-range ordering in Pd₄₀Ni₄₀P₂₀ bulk metallic glasses — ●MANOEL WILKER DA SILVA PINTO, MARK STRINGE, DRAŽEN RADIĆ, HARALD RÖSNER, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Individual annealing treatments at $0.8T_g$ and $0.9T_g$ on Pd₄₀Ni₄₀P₂₀ bulk metallic glass samples were performed in a differential scanning calorimeter to either activate mainly β or both α and β relaxation processes. Prior to and after these measurements the samples were heated into the supercooled liquid in order to establish a comparable reference relaxation state.

The medium-range order of the different stages of the amorphous structures were investigated by fluctuation electron microscopy and compared with that of the as-cast state. The results indicate that first, a defined structural reset was achieved when heating into the supercooled liquid; however, with increased strain due reduction of excess volume. Second, the annealing treatment at $0.8T_g$ increases the volume fraction of medium-range order again with annealing time and third, a depletion of the volume fraction is observed after annealing at $0.9T_g$.

MM 28.2 Wed 10:30 SCH A 118

Analysis of the relaxational behavior of PdNiS — ●MAXIMILIAN DEMMING¹, NICO NEUBER², MARTIN PETERLECHNER¹, RALF BUSCH², and GERHARD WILDE¹ — ¹University of Münster, Münster, Germany — ²Saarland University, Saarbrücken, Germany

In this work we examine a sulfur-containing bulk metallic glass, PdNiS. The impact of sulfur is investigated with a focus on the thermodynamic behavior and the comparison with the well-known PdNiP bulk metallic glass. Several samples from the same initial state were annealed at a certain temperature below T_g for different annealing times in order to adjust distinct relaxation states. After isothermal annealing in a differential scanning calorimeter (DSC), a calorimetric study was carried out to examine the relaxation behavior. Especially the so-called overshoot during heating the samples through the glass transition was evaluated, since it is one of the most prominent signals which depends on the thermal history of a metallic glass. Additionally, low temperature heat capacity measurements were performed to quantify the so-called boson peak. The boson peak can be related to soft vibrational modes, and thus it is characteristic to the relaxational state of a metallic glass and it is affected by the thermal history of a glass. All methods combined deliver a picture of the relaxational behavior under pre- T_g annealing of this Sulphur-containing metallic glasses.

MM 28.3 Wed 10:45 SCH A 118

Unravelling the origin of the anomalous thermal expansion in Fe-based bulk metallic glasses — ●ALEXANDER FIRLUS¹, MIHAI STOICA¹, GAVIN VAUGHAN², STEFAN MICHALIK³, ROBIN E. SCHÄUBLIN¹, and JÖRG F. LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, ETH Zurich, 8093 Zurich, Switzerland — ²European Synchrotron Radiation Facility (ESRF), Grenoble, France — ³Diamond Light Source Ltd., Didcot, UK

Fe-based bulk metallic glasses (BMGs) are known for their soft-magnetic properties but their magnetic interactions also give rise to an anomalous thermal expansion, called the Invar effect. In the ferromagnetic state, their coefficient of thermal expansion is reduced by a factor of four. This phenomenon has been observed in all ferromagnetic Fe-based BMGs at the macroscopic scale, but due to the lack of long-range order the physics of this effect needs to be described at the atomic scale. Although it is now widely accepted to be of magnetic origin, the contributions of the different atomic species to the Invar effect have been unknown. We studied the atomic-scale thermal expansion of multiple quaternary BMGs by in situ X-ray diffraction. The anomalous thermal expansion is visible in all diffraction patterns and can clearly be associated with the disordered Fe network. Through variations of the minor alloying elements, we elucidated the effect of different atomic species and provide a framework in which their respective influence on the Invar effect can be understood.

MM 28.4 Wed 11:00 SCH A 118

Rejuvenation engineering in metallic glasses by complementary stress and structure modulation — ●DANIEL ŞOPU^{1,2}, FLORIAN SPIECKERMANN³, SIMON FELLNER¹, CHRISTOPH GAMMER¹, and JÜRGEN ECKERT^{1,3} — ¹Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria — ²Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — ³Department of Materials Science, Chair of Material Physics, Montanuniversität Leoben, Austria

Residual stress engineering is very widely used in the design of new advanced lightweight materials. For metallic glasses the attention has been on structural changes and rejuvenation processes. Here, based on high energy scanning X-ray diffraction strain mapping, transmission electron microscopy (TEM) and microindentation we distinguish between structural and elastic fluctuations, the two key factors for the observed extreme rejuvenation in triaxial compression. TEM characterization shows that structural rejuvenation under room temperature deformation relates to shear-induced softening and dilatation (large volumetric strain). High energy scanning X-ray diffraction strain mapping reveals large elastic fluctuations in metallic glasses after deformation under triaxial compression. Microindentation hardness mapping hints to a competing hardening-softening mechanism after compression and further reveals the complementary effects of stress and structure modulation. Molecular dynamics simulations provide an atomistic understanding of the complex shear band activity in notched metallic glasses and the related fluctuations in the strain/stress heterogeneity.

MM 28.5 Wed 11:15 SCH A 118

Enhancing mechanical properties by introducing surface grooves in metallic glasses — ●XUDONG YUAN¹, DANIEL ŞOPU^{1,2}, KAIKAI SONG³, and JÜRGEN ECKERT^{1,4} — ¹Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, Leoben A-8700, Austria — ²Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Otto-Berndt-Str.3, Darmstadt D-64287, Germany — ³School of Mechanical, Electrical and Information Engineering, Shandong University (Weihai), Weihai 264209, China — ⁴Department of Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, Leoben A-8700, Austria

The correlation between the mechanical properties and surface defects in metallic glasses (MGs) is investigated by surface ultrasonic bonding experiments and molecular dynamics simulations. The strength together with the compression ductility of Zr₆₅Cu₁₅Ni₁₀Al₁₀ MG can be enhanced by introducing surface grooves. Induced grooves and pre-shear bands (SBs) lead to the formation and interaction of multiple SBs during compression, which consequently enhances ductility. Additionally, the thermal-induced nanocrystallization, together with generated free volume and residual stresses around the grooves contribute to the emergence of hierarchical structure and stress heterogeneity, which delays the propagation of dominant SB and enables the improvement of strength and plasticity of MG.

15 min. break

MM 28.6 Wed 11:45 SCH A 118

Atomic transport in heavy ion irradiated amorphous PdNiP near the glass transition temperature — ●SABA KHADEMOREZAIAN¹, MARILENA TOMUT^{1,2}, MAXIMILIAN DEMMING¹, 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

The influence of ion irradiation on Ag diffusion in Pd₄₀Ni₄₀P₂₀ bulk metallic glass was investigated by the tracer diffusion technique at temperatures below the glass transition. Bulk samples of Pd₄₀Ni₄₀P₂₀ relaxed states were irradiated with 4.8 MeV/u Au, U, and Ca ions at the UNILAC accelerator at GSI Darmstadt. The achieved fluences were in the range of 5×10^{10} to 1×10^{13} ions/cm². The diffusion rates of ^{110m}Ag isotopes after irradiation with heavy ions, Au and U, were found to be monotonously increasing with increasing total fluence. For the light ions, Ca, the diffusion enhancement shows an unexpected non-monotonous, cross-over behavior. The results are discussed re-

lating the impacts of irradiation with swift heavy ions on structure modifications and the atomic kinetics in a bulk metallic glass.

MM 28.7 Wed 12:00 SCH A 118

Nanostructural investigations on thin film nanoglasses using different TEM techniques — ●HENDRIK VOIGT¹, EVGENIY BOLTYNJUK², AARON RIGONI¹, HORST HAHN², HARALD RÖSNER¹, and GERHARD WILDE¹ — ¹University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Karlsruhe Institute of Technology, Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Nanoglasses as a relatively new family of amorphous alloys present an attempt to tailor the structure of glasses to improve their properties. The concept of nanoglasses is based on the introduction of glass-glass interfaces into the amorphous material, mimicking the effect that defects have in crystalline matter. Different transmission electron microscopy (TEM) techniques were used to investigate the microstructure of Cu₆₀Zr₄₀ columnar thin film nanoglasses. Nanobeam diffraction pattern (NBDP) analysis and energy dispersive X-ray spectroscopy (EDX) were employed to investigate differences in the excess free volume and chemical composition. NBDP acquired over an extended region of interest were used to perform an angular correlation analysis revealing different symmetry motives compared to a compositionally equivalent homogenous glass. Additionally, time-of-flight secondary ion mass spectroscopy (ToF SIMS) measurements discovered an increase in diffusivity in the nanoglasses. All the results shown here provide clear evidence for the existence of glass-glass interfaces with two structurally different phases present in the nanoglass.

MM 28.8 Wed 12:15 SCH A 118

Properties of Sodium Borosilicate Glasses via Dynamics Simulations with Ultra-Fast Machine-Learning Potentials — ●HENDRIK KRASS¹, BENEDIKT ZIEBARTH², WOLFGANG MANNSTADT², and MATTHIAS RUPP³ — ¹University of Konstanz, Konstanz, Germany — ²Schott AG, Mainz, Germany — ³Luxembourg Institute of Science and Technology (LIST), Belvaux, Luxembourg

Glasses are of scientific interest and have many industrial applications.

However, their investigation and development are limited by the duration and costs of experiments. The computational study of glasses can in principle overcome these limits, but current atomistic glass models are either fast but not accurate enough (classical empirical potentials) or accurate but too slow (ab initio potentials). Machine-learning potentials (MLPs) trained on ab initio reference calculations promise to be both fast and accurate enough.

We investigate the suitability of “ultra-fast potentials” (UFPs) [1]—a class of MLPs that are data-efficient, physically interpretable, sufficiently accurate for applications, can be parametrized automatically, and are as fast as the fastest traditional empirical potentials—to study glasses. For this, we compute structure and properties of interest via dynamics simulations with UFPs and compare them against state-of-the-art models and experimental values for sodium borosilicate glasses, a prototypical glass system.

[1] Stephen R. Xie, Matthias Rupp, Richard G. Hennig: Ultra-Fast Interpretable Machine-Learning Potentials, arXiv 2110.00624, 2021.

MM 28.9 Wed 12:30 SCH A 118

An atomic scale inspired phase-field approach to model fracture in amorphous silica — ●GERGELY MOLNAR¹, GAYLORD GUILLOMNEAU², GUILLAUME KERMOUCHE³, and ETIENNE BARTHEL⁴ — ¹Univ Lyon, CNRS, INSA Lyon, LaMCoS, UMR5259, 69621 Villeurbanne, France — ²Univ Lyon, Ecole Centrale de Lyon, CNRS, LTDS, UMR CNRS 5513, 69134 Ecully, France — ³Mines Saint-Etienne, CNRS, UMR 5307 LGF, Centre SMS, 42023 Saint Etienne, France — ⁴ESPCI, CNRS, SIMM, UMR7615, 75231 Paris, France

In the last decade, phase-field models have gained great popularity in fracture simulation. These models regularize the sharp crack using an internal length-scale by diffusing the damage into the material. This work was set out to investigate the competition between homogeneous plastic deformation, shear banding, and brittle failure in amorphous silica. The molecular dynamics inspired finite element model uses the phase-field approach to model fracture, while a pressure-dependent yield criterion accounts for densification and shear plasticity. The talk presents a proof of concept to model plasticity and crack propagation in micrometer size silica samples.

MM 29: Data Driven Materials Science: Big Data and Work Flows – Electronic Structure

Time: Wednesday 11:45–13:00

Location: SCH A 251

MM 29.1 Wed 11:45 SCH A 251

Band Gap and Formation Energy Inference of Solids using Message Passing Neural Networks — ●TIM BECHTEL, DANIEL SPECKHARD, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Berlin, Germany

Graph-based neural networks and, specifically, message-passing neural networks have shown great promise in predicting physical properties of solids. Here, we target three tasks, formation energy regression, metal-non-metal classification, and band gap regression, using data from the AFLOW materials database [1]. In order to find optimal hyperparameters and model architecture, we perform a neural architecture search on the band gap regression task, using a random search algorithm. The model is based on a message passing neural network with edge updates [2], and provides users with uncertainty estimates via Monte-Carlo dropout. We analyze the domain of applicability of the model, for different space group symmetries, atomic species, and corrections applied to the underlying calculation. While we obtain overall excellent results, the model struggles to accurately predict oxide materials. We find that the uncertainty in different domains reflects the model’s predictive performance.

[1] S. Curtarolo et al., *Comput. Mater. Sci.*, 58 (2012), pp. 227-235.

[2] P.B. Jørgensen et al., Preprint at arXiv:1806.03146 (2018).

MM 29.2 Wed 12:00 SCH A 251

Predicting electron density using a convolutional neural network — ●JAE-MO LIHM^{1,2,3}, WANHEE LEE⁴, and CHEOL-HWAN PARK^{1,2,3} — ¹Department of Physics and Astronomy, Seoul National University, Seoul, Korea — ²Center for Correlated Electron Systems, Institute for Basic Science, Seoul, Korea — ³Center for Theoretical Physics, Seoul National University, Seoul, Korea — ⁴Department of Applied Physics, Stanford University, California, USA

Machine-learning methods are being widely applied to computational materials science. Most applications of machine learning in electronic structure calculations focus on learning the total energy and forces, while few works study the prediction of electronic properties. In this work, we develop a machine-learning model for predicting electron density using the convolutional neural network, a standard machine-learning method for image processing. We train the neural network using the electron density calculated from density functional theory. We show that the trained neural network can successfully predict the electron density of systems that were not included in the training set, bypassing the need for the self-consistent density functional theory calculation.

MM 29.3 Wed 12:15 SCH A 251

Chemical ordering and magnetism in CrCoNi Medium Entropy Alloy — ●SHEULY GHOSH¹, VADIM SOTSKOV², ALEXANDER SHAPEEV², JÖRG NEUGEBAUER¹, and FRITZ KÖRMANN^{1,3} — ¹Max-Planck-Institut für Eisenforschung GmbH — ²Skolkovo Institute of Science and Technology — ³Delft University of Technology

The equiatomic CrCoNi medium entropy alloy is a prototypical multiple-principal element alloy (MPEA), exhibiting many superior mechanical properties. Short-range order (SRO) is known to affect the thermodynamic phase stability as well as mechanical and magnetic properties of MPEA alloys. In CrCoNi also, the presence of SRO and its impact on different aspects has been intensively discussed in various studies. In our recent study, we identified the ground-state ordered structure for this alloy combining *ab initio* calculations and on-lattice machine-learning interatomic potentials. Based on these studies, an ordered Cr(Ni,Co)₂ phase (MoPt₂-type) was found. In present work, we further discuss the stability of the newly identified ordered structure and compare them with the previously suggested ones, particularly with respect to magnetism, local atomic relaxation energies as well as

volume fluctuations.

MM 29.4 Wed 12:30 SCH A 251

Charge-dependent Atomic Cluster Expansion — ●MATTEO RINALDI, ANTON BOCHKAREV, YURY LYSOGORSKIY, MATOUS MROVEC, and RALF DRAUTZ — Interdisciplinary Centre for Advanced Materials Simulation, Bochum, Germany

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 outperforming popular approaches based on limited body-order descriptions. However, due to the local nature of the many body basis, it is inherently near-sighted. Therefore, long range interactions, such as electrostatics, are ignored in the description. Here, we introduce charge-dependent ACE to be able to tackle the missing electrostatic contributions. This formalism is based on the QEQ charge equilibration scheme from Rappe et al. [4], where partial charges are obtained by equalizing atomic electronegativities and imposing charge conservation. Moreover, atomic electronegativities and hardness are considered as dependent on the local atomic environment. We demonstrate that our approach yields atomic charges in agreement with those obtained from popular partitioning schemes, such as Mulliken and Hirshfeld, including periodic and non-periodic systems, together with an accurate reproduction of the potential energy landscape. This work opens the possibility to model charge transfer and dielectric response within the increasingly popular ACE framework.

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

[4] Rappe, J. Phys. Chem. 1991, 95, 8, 3358*3363

MM 29.5 Wed 12:45 SCH A 251

A machine-learned interatomic potential for silica and mixed silica-silicon systems — ●LINUS C. ERHARD¹, JOCHEN ROHRER¹, KARSTEN ALBE¹, and VOLKER L. DERINGER² — ¹Institute of Materials Science, TU Darmstadt, Darmstadt, Germany — ²Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, United Kingdom

The interface between silica and silicon has enormous relevance in various applications, including semiconductors and novel battery materials. However, atomistic modeling of this interface is a challenge due to the different charge states of silicon and the limitations of classical interatomic potentials. To overcome these limitations, we introduce a machine-learning-based interatomic potential based on the non-linear atomic cluster expansion (ACE) for various Si-O phases. This model is based on the previously developed database for silica [1], which was substantially extended by active learning. The new model shows improved performance for high-pressure silica and is also able to describe silica surfaces. Moreover, the use of the ACE formalism enables us to reach more than 100 times longer time or larger length scales compared to the Gaussian approximation potential (GAP). Finally, the potential is able to describe off-stoichiometric mixtures of Si and SiO₂. This capability is used to investigate the nanostructure of silicon monoxide.

[1] Erhard et al. A machine-learned interatomic potential for silica and its relation to empirical models. npj Comput Mater 8, 90 (2022)

MM 30: Invited Talk: Liebscher

Time: Wednesday 15:00–15:30

Location: SCH A 251

Invited Talk

MM 30.1 Wed 15:00 SCH A 251

Direct observations of grain boundary phase transformations in metallic alloys — ●CHRISTIAN LIEBSCHER — Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany

Grain boundaries (GBs) play a pivotal role in determining the properties of metallic materials. In most considerations, GBs are seen as a simple 2D defect. However, thermodynamic concepts already proposed 60 years ago showed that GBs can undergo phase transformations, but the search for them has been in vain due to their confined nanoscale nature.

We show that GB phases exist in elemental copper. Atomic resolu-

tion scanning transmission electron microscopy is used to unravel multiple coexisting GB structures in the same GB. The intrinsic character and thermodynamic properties of the GB phases and their transitions is investigated by atomistic simulations. We find that the GB phase junction, a line defect that separates different GB phases, is kinetically limiting the transformation and plays a decisive role in the nucleation and arrangement of GB phases within the interface. By heating GBs inside of the electron microscope, we are able to directly observe how GB phases evolve at elevated temperatures with atomic resolution. In the remainder of the talk, we will also discuss the impact of solute segregation on GB transitions in copper and titanium alloys by exploring the local atomic arrangement of solutes within the GB.

MM 31: Data Driven Materials Science: Big Data and Work Flows – Machine Learning

Time: Wednesday 15:45–18:30

Location: SCH A 251

MM 31.1 Wed 15:45 SCH A 251

Neural networks trained on synthetically generated crystals can classify space groups of ICSD powder X-ray diffraction patterns — ●HENRIK SCHOPMANS, PATRICK REISER, and PASCAL FRIEDERICH — Institute of Theoretical Informatics, KIT, Karlsruhe, 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 types. 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 77.4% on new ICSD structure types 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, such as 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.

MM 31.2 Wed 16:00 SCH A 251

Critical Assessment of Uncertainty Estimates of Machine-Learning Potentials — ●SHUAHUA LU^{1,2}, LUCA M. GHIRINGHELLI¹, CHRISTIAN CARBOGNO¹, and MATTHIAS SCHEFFLER¹ — ¹Novel Materials Discovery at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin, Berlin, Germany — ²School of Physics, Southeast University, Nanjing, China

Machine-learning potentials (MLP) trained on first-principles datasets are becoming increasingly popular since they enable the treatment of larger system sizes and longer time scales compared to straight ab initio techniques. A key aspect for the use of these MLPs is to reliably assess the accuracy viz. uncertainty of the predictions, e.g., by training an ensemble of models. Here, we critically examine the robustness of such uncertainty predictions using equivariant message-passing neural networks as an example [1]. We train an ensemble of models on liquid silicon simulated at the gradient-corrected density-functional-theory level and compare the predicted uncertainties with actual errors for various test sets, including liquid silicon at different temperatures and out-of-training-domain data such as solid phases with and without point defects as well as surfaces. These studies reveal that the pre-

dicted uncertainties are often overconfident. This is ascribed to the insufficient diversity in the members of the ensemble, as measured via error correlations. [1] S. Batzner et al., Nat. Commun. 13, 2453 (2022).

MM 31.3 Wed 16:15 SCH A 251

Learning to Spell Materials - Coordinate-free Discovery with Natural Language Processing — ●KONSTANTIN JAKOB, KARSTEN REUTER, and JOHANNES T. MARGRAF — Fritz Haber Institute, Berlin, Germany

Over the last decade, computational screening with structure-based machine learning models has led to some advances in the discovery of novel inorganic materials. Unfortunately, the overwhelmingly large space of possible compositions and atomic configurations together with the exceeding rarity of well-suited candidates ultimately poses a limit to the applicability of this approach. In contrast, purely composition-based representations neglect differences in the chemical properties of different crystal polymorphs and thus lack accuracy. A middle ground between full structural and simple compositional representations has been established for organic molecules using string representation such as SMILES. While these have proven highly advantageous for molecular discovery when combined with natural language processing models, analogous representations for the more complex class of inorganic materials are still missing. Bridging this gap, we investigate the performance of recurrent neural networks (RNNs) in predicting crystallographic properties by reading a materials composition element by element. Their striking accuracy suggests that symmetry- or prototype-based string representations could be generated with little computational effort at a large scale. The invertibility of these intermediate representations via restricted structure searches is investigated, paving the way to their application for conditional generative models.

MM 31.4 Wed 16:30 SCH A 251

Exploring materials dataspace by combining supervised and unsupervised machine learning — ●ANDREAS LEITHERER¹, ANGELO ZILETTI¹, CHRISTIAN H. LIEBSCHER², TIMOFEY FROLOV³, and LUCA M. GHIRINGHELLI^{1,4} — ¹NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität (HU) zu Berlin — ²Max-Planck-Institut für Eisenforschung — ³Lawrence Livermore National Laboratory — ⁴Physics Department and IRIS-Adlershof of HU zu Berlin

To enable meaningful applications of AI to materials science, much of current efforts is concentrated on the creation of characterized datasets. In this talk, we discuss a rarely addressed topic - the development of automatic tools to explore available materials-science data. In particular, we go beyond purely supervised learning by combining unsupervised analysis with a recently developed crystal-structure recognition method [1]. This neural-network (NN) model automatically learns data representations that contain information on structurally diverse geometries. Using clustering, physically meaningful subgroups can be identified in the NN latent space, which are shown, e.g., to correspond to distinct, experimentally verified grain-boundary phases [2]. Moreover, dimension-reduction analysis allows us to create low-dimensional, interpretable materials charts that visualize complex structural data from both theoretical and experimental origin.

[1] A. Leitherer, A. Ziletti and L. M. Ghiringhelli. Nat. Commun. 12, 6234 (2021)

[2] T. Meiners et al. Nature 579, 375-378 (2020)

MM 31.5 Wed 16:45 SCH A 251

Minimizing data requirements by transfer learning for structure search on organic/inorganic interfaces — ●ELIAS FÖSLEITNER, JOHANNES CARTUS, LUKAS HÖRMANN, and OLIVER T. HOFMANN — Institute of Solid State Physics, Graz University of Technology, Graz, Austria

Performing structure search of organic molecules on metallic surfaces requires finding the structure with the lowest energy. However, calculating energies using conventional DFT codes proves to be a time-consuming task since single calculations are expensive and the number of configurations is large. To avoid the calculation of all possible structures, machine learning techniques such as Gaussian process regression have shown to be a useful tool in order to reduce the amount of DFT data needed. In our work we try to further reduce the amount of necessary data by using transfer learning from one substrate to another. To do this we include DFT data from structures of more than one substrate in our training set. In order to calculate the similarities between structures on different substrates we use the SOAP descriptor combined with an alchemical kernel which provides couplings between

the different substrate elements. By optimizing these couplings, although molecule-substrate interactions differ notably (e.g. the interfacial charge transfer) between different substrates, we can save up to 50 % of the training data for one substrate A by also using the data of another substrate B. This serves as a stepping stone for the investigation of structures on computationally costly substrates.

15 min. break

MM 31.6 Wed 17:15 SCH A 251

Accelerating the Search for High-Performance, Novel Materials with Active Learning — ●THOMAS A. R. PURCELL¹, MATTHIAS SCHEFFLER^{1,2}, LUCA M. GHIRINGHELLI^{1,2}, and CHRISTIAN CARBOGNO¹ — ¹The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin — ²Physics Department and IRIS-Adlershof at Humboldt Universität zu Berlin, Berlin, Germany.

Active-learning frameworks have the potential to greatly accelerate the search for new materials. By balancing exploitation and exploration, these approaches can efficiently search through materials space and find the regions that are most likely to contain promising candidate materials [1]. Here we present an active learning framework, that uses an ensemble of expressions found by the sure-independence screening and sparsifying operator (SISSO) approach [2,3], and we demonstrate it for the example of discovering new thermal insulators. We statistically process the predictions of independent SISSO models to automatically select the most promising material candidates and then calculate their thermal conductivity κ_L using the *ab initio* Green Kubo method [4]. Using this approach we are able to find multiple new thermal insulators and gain insights into what is driving down their κ_L .

[1] A. G. Kusne, et al. Nat. Comm. 11, 5966 (2020)

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

[3] T. A. R. Purcell, et al. J. Open Source. Softw. 7, 3960 (2022)

[4] F. Knoop, et al. arXiv:2209.12720

MM 31.7 Wed 17:30 SCH A 251

Machine learning discovery of new materials — ●JONATHAN SCHMIDT^{1,2}, HAI-CHEN WANG², NOAH HOFFMAN², TIAGO CERQUEIRA³, PEDRO BORLIDO³, PEDRO CARRICO³, LOVE PETTERSSON⁴, CLAUDIO VERDOZZI⁴, SILVANA BOTTI¹, and MIGUEL MARQUES² — ¹Friedrich-Schiller-University Jena, Germany — ²Martin-Luther-University Halle-Wittenberg, Germany — ³University of Coimbra, Portugal — ⁴Lund University, Sweden

Graph neural networks for crystal structures typically use the atomic species and atomic positions as input. We construct crystal-graph attention networks replacing these precise bond distances with embeddings of graph distances. This allow us to perform high-throughput studies based on both compositions and crystal structure prototypes. Combining a newly curated dataset of 3M materials and the networks we have already scanned more than two thousand prototypes spanning a space of more than 5 billion materials and identified tens of thousands of theoretically stable compounds. We also demonstrate the effectiveness of transfer learning to adapt the networks to new domains such as of two dimensional structures.

Schmidt et al. Crystal graph attention networks for the prediction of stable materials, Sci. Adv. 7.49 (2021)

Schmidt et al., Large-scale machine-learning-assisted exploration of the whole materials space, arXiv:2210.00579 (2022)

Wang et al., Symmetry-based computational search for novel binary and ternary 2D materials, submitted (2022)

MM 31.8 Wed 17:45 SCH A 251

Data-driven magneto-elastic interatomic potentials for discovering novel phases of transition metal alloys — ●MANI LOKAMANI¹, KUSHAL RAMAKRISHNA⁴, JULIAN TRANCHIDA³, SVETOSLAV NIKOLOV², HOSSEIN TAHMASBI⁴, MICHAEL WOOD², and ATTILA CANGI⁴ — ¹HZDR Dresden, Germany — ²SNL New Mexico, USA — ³CEA Cadarache, France — ⁴CASUS Görlitz, Germany

Structural prediction methods are used for identifying stable and metastable structures in a broad spectrum of materials. The presence of the electron spin degree of freedom in magnetic materials increases the complexity of finding such structures, constraining the analysis to the thermodynamically most relevant structures in a narrow range of temperatures and pressures. We achieve a search over much wider temperature and pressure conditions by utilizing machine-learning interatomic potentials based on the spectral neighbor analysis

method within the coupled spin-molecular dynamics framework implemented in LAMMPS. This data-driven methodology enables predicting the properties of magnetic materials on much larger spatial, spin, and temporal domains and is parametrized by first-principles data. Leveraging this methodology, we predict the formation of metastable crystalline structures in transition metal alloys (FeNi, FeMn, FeCr, FeCo, FeGd) at high temperature-pressure conditions and assess their magnetic properties. This enables studying long-range spin structures in novel phases of transition metal alloys and complements the quest for permanent magnets for renewable energy applications that do not depend on rare-earth elements.

MM 31.9 Wed 18:00 SCH A 251

FAIR Modelling Recipes for High-Throughput Screening of Metal Hydrides — •KAI SELLSCHOPP¹, PHILIPP ZSCHUMME², MICHAEL SELZER², CLAUDIO PISTIDDA¹, and PAUL JERABEK¹ — ¹Institute for Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — ²IAM - Microstructure Modelling and Simulation, Karlsruhe Institute of Technology, Karlsruhe, Germany

A simple modelling recipe for calculating the hydrogenation enthalpy of metal hydrides with ab-initio methods is presented. It consists of the everyday tasks of a computational materials scientist: relaxing a structure, optimising its volume, and calculating vibrational energies. The corresponding workflow is implemented in the framework of KadiStudio^[1], where the scientific process is broken down into simple input-processing-output (IPO) tasks. The approach allows to track the inputs and outputs, to easily re-use the modular tasks in other workflows, and to share the workflow as a simple bash or python script. Therefore, not only the generated research data, but also the workflow itself fully comply with the FAIR data principles. As a first application, the recipe is employed to test how the different ingredients of an ab-initio calculation (e.g. xc-functional) affect the accuracy of pre-

dicting hydrogenation enthalpies. This helps to make better choices for studying this class of materials in the future and to judge the uncertainty in existing data. Furthermore, the standardized workflow enables a reliable high-throughput screening of new candidate materials for high-density hydrogen storage at near ambient conditions.

[1] L. Griem, *et al.*, Data Science Journal **21**, 16 (2022)

MM 31.10 Wed 18:15 SCH A 251

Take Two: Δ -Machine Learning for Molecular Co-Crystals — •SIMON WENGERT¹, GÁBOR CSÁNYI², KARSTEN REUTER¹, and JOHANNES THEO MARGRAF¹ — ¹Fritz-Haber Institute, Berlin, Germany — ²University of Cambridge, Cambridge, United Kingdom

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 as demonstrated via molecular dynamics simulations at ambient conditions.

MM 32: Topical Session: Defect Phases I

Time: Wednesday 15:45–18:30

Location: SCH A 216

Topical Talk MM 32.1 Wed 15:45 SCH A 216
Defect phase diagrams: Concepts, computational approaches and applications — MARVIN POUL, PRINCE MATHWS, ALI TEHRANCHI, JING YANG, MIRA TODOROVA, TILMANN HICKEL, and •JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Extending the well-known concept of bulk phase diagrams to defects allows to predict the thermodynamically stable defect states at any given temperature and bulk composition. Similar to bulk phase diagrams such diagrams allow to identify processing conditions where defect states with particularly desirable stoichiometries, structures and properties form. These diagrams thus provide an exciting new approach in designing materials. Modern atomistic tools based on density functional theory or machine learning potentials can provide all the necessary information to construct such phase diagrams but face severe conceptual and computational challenges: The description of such defects requires thermodynamically open boundary conditions as well as the inclusion of a large number of structural, chemical and electronic degrees of freedom. In the presentation, key concepts of efficiently sampling the large configuration spaces associated with computing defect states and phase diagrams will be discussed. Examples of how this insight can be used to understand and control grain boundary formation, morphology or improved corrosion resistance will be given.

MM 32.2 Wed 16:15 SCH A 216

Fully Automated Calculation of Defect Phase Diagrams — •MARVIN POUL, ERIK BITZEK, and JOERG NEUGEBAUER — Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Deutschland

Understanding the thermodynamics of segregation at crystal defects is an important part of successful materials engineering.[1] We present an efficient method that constructs finite temperature Defect Phase Diagrams (DPDs) for binary alloys from fully relaxed molecular calculations using machine learning interatomic potentials (MLIP) without user intervention and implemented it as a pyiron[2] workflow. A major challenge that we had to address is the combinatorially growing number of different segregation configurations at any extended defect. The proposed method is able to efficiently tackle hundreds of thousands to

millions of configurations and is based on a fast proxy model. This model is based on the ACE descriptors and avoids having to evaluate a full MLIP. This proxy model together with the MAXVOL active learning algorithm allows to pre-screen which configurations to calculate with the underlying MLIP. We apply the workflow on the example of Al and Ca segregation to Mg grain boundaries.

[1]: Korte-Kerzel, S. et al. (2022) Defect phases: thermodynamics and impact on material properties, International Materials Reviews, 67:1, 89-117

[2]: Janssen, J, et al. "pyiron: An integrated development environment for computational materials science." Computational Materials Science 163 (2019): 24-36.

MM 32.3 Wed 16:30 SCH A 216

Effect of chemical changes on the defect structures in lean rare-earth free ternary Mg alloys — •WASSILIOS DELIS¹, DEBORAH NEUSS², MARCUS HANS², DIERK RAABE³, SANDRA KORTE-KERZEL¹, and STEFANIE SANDLÖBES-HAUT¹ — ¹Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Germany — ²Materials Chemistry, RWTH Aachen University, 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 sufficient 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. Alloys containing low amounts of Al and Ca showed a highly increased room temperature ductility. Here, TEM and APT measurements and ab initio calculations showed an increased activity of $\langle c+a \rangle$ dislocation slip. The effects of the alloying elements are yet not fully understood. Further research has been performed to investigate how the changes in chemistry affect the structure of defects such as boundaries and dislocations.

MM 32.4 Wed 16:45 SCH A 216

High-throughput generation of defect phase diagrams: A case study in grain boundary solute segregation analysis in Ni base alloys — •HAN LIN MAI, TILMANN HICKEL, and JÖRG NEUGEBAUER

— Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Understanding segregation to grain boundaries, and eventually their defect phase diagrams, is critical to enable rational grain boundary engineering for alloys design. Here, we discuss the progress and challenges one may face when generating such a database of defect-solute interactions, in the context of studying of grain boundary segregation of solutes and impurities in Ni GBs. To compute the large number of relevant defect-solute interactions we have performed high-throughput ab initio calculations using efficient and highly automated workflows using pyiron. The study has been performed across a representative set of coincident-site-lattice (CSL) type tilt GBs. Based on the large ab-initio datasets, we extract and analyse the chemical and structural trends observed in the solute segregation behaviour across the periodic table. The features which are most important in evaluating site segregation are presented and discussed.

15 min. break

MM 32.5 Wed 17:15 SCH A 216

Planar defects in intermetallic $Mg_xAl_{2-x}Ca$ Laves phases — ●ALI TEHRANCHI¹, TILMANN HICKEL^{1,2}, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — ²Bundesanstalt für Materialforschung und -prüfung (BAM)

The intermetallic Laves phases that are present in Mg-based alloys when adding Ca and Al beyond the solubility limit have a beneficial impact on the mechanical properties of these alloys. For example, Laves phases have been observed to enhance the alloy's creep resistance and to extend their application to higher-temperature domains. However, the mechanism of deformation of these phases and their effect on the surrounding matrix is not fully understood. Laves phases not only contain planar defects but also their motifs are observed in planar defects in Mg. In this work, using the concept of defect phase diagrams, we study hcp-like planar defects in the C36 phase and the thermodynamically stable Laves-type planar defects in Mg-based alloys. We show, that while conventional bulk thermodynamic phase diagrams fail to predict the experimentally observed phases the predictions obtained by the defect phase diagrams match well with the experiments. Defect phase diagrams thus provide a powerful tool to predict and interpret the formation of chemically and structurally complex motives at defects as function of experimentally accessible and controllable parameters such as temperature or alloy composition.

MM 32.6 Wed 17:30 SCH A 216

Oxygen vacancy formation energies at grain boundaries in perovskite-type electro-ceramics — ●CONG TAO¹, DANIEL MUTTER¹, DANIEL F. URBAN^{1,2}, and CHRISTIAN ELSÄSSER^{1,2} — ¹Fraunhofer IWM, 79108 Freiburg — ²Freiburg Materials Research Center (FMF), University of Freiburg, 79104 Freiburg

Oxygen vacancy concentrations are assumed to play a major role in the electric-field assisted grain growth of technologically relevant single crystal perovskite phases. The underlying effect on the atomic scale is the redistribution of cationic and anionic point defects between grain boundaries and bulk phases due to different defect formation energies in the structurally different regions, accompanied by the formation of space charge zones. In this study, we present results of clas-

sical atomistic calculations of oxygen vacancy formation energy profiles across supercells containing the symmetric tilt grain boundaries $\Sigma 5(210)[001]$, $\Sigma 5(310)[001]$, and the asymmetric tilt grain boundary $(430) \parallel (100)$. The electro-ceramic perovskite materials $SrTiO_3$, $BaTiO_3$, and $BaZrO_3$ were systematically analyzed. We discuss the dependence of formation energies and resulting concentration profiles on composition and grain boundary type.

MM 32.7 Wed 17:45 SCH A 216

Temperature-dependent impact of antiphase boundaries on properties of Fe_3Al — ●MARTIN FRIÁK^{1,2}, MIROSLAV ČERNÝ^{2,3}, and MOJMÍR ŠOB^{4,1} — ¹Institute of Physics of Materials, Czech Academy of Science, Brno, CZ — ²Central European Institute of Technology (CEITEC), Brno University of Technology, Brno, CZ — ³Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — ⁴Department of Chemistry, Faculty of Science, Masaryk University, Brno, CZ

We have performed a quantum-mechanical study of the influence of antiphase boundaries (APBs) on the temperature dependence of selected materials properties of Fe_3Al . We show that the studied APBs very strongly affect thermal vibrations of Fe_3Al and reduce the width of the band gap in phonon frequencies. Our results also show that the Fe_3Al with APBs exhibits higher volumetric thermal expansion than the defect-free Fe_3Al . The computed free energy of APBs is found to be strongly temperature-dependent. It is lower than the static-lattice temperature-independent APB energy and the reduction is enhanced by increasing temperature (to 76% at $T = 700$ K). We have also addressed the discrepancy between the experimental bulk modulus and previous theoretical results obtained for the defect-free Fe_3Al . Due to the presence of APBs, the bulk modulus is reduced from the value of 173 GPa, that corresponds to the defect-free Fe_3Al , to 153 GPa, i.e. very close to the experimental value of 147 GPa (at $T = 0$ K). For details see *Intermetallics* 151 (2022) 107746, DOI:10.1016/j.intermet.2022.107746.

MM 32.8 Wed 18:00 SCH A 216

Towards a Rigorous Theory of Grain Boundary Segregation in Polycrystals — ●CHRISTOPHER SCHUH — MIT, Department of Materials Science and Engineering, Cambridge, MA USA

Although grain boundary segregation is pervasive across metals and materials, the models used to describe it generally fall short in one of two ways. One class of models is too approximate, using, e.g., a scalar 'average' segregation energy; the other is too detailed, focusing on specific atomic sites in select boundaries. Both approaches fail to capture the complex range of sites in the grain boundary network of polycrystals. This talk will overview a project in our group at MIT that aims to develop a new type of grain boundary segregation theory that bridges this gap: it is designed to be quantitatively accurate at the level of specific grain boundary sites, but simple enough to admit solution with an isotherm that can be analytically represented. The approach is based on the parameterization of segregation spectra: distribution functions of all the key thermodynamic quantities necessary to capture the full physics of segregation in polycrystals. We address the spectra of: segregation sites and their enthalpies, interaction parameters amongst solutes, and vibrational contributions to the segregation free energy. After describing computational methods to determine these spectra, we then address the problem of high-throughput computation of them for many alloy systems using tools of data science.

MM 33: Topical Session: Fundamentals of Fracture – Amorphous Metals

Time: Wednesday 15:45–18:00

Location: SCH A 215

MM 33.1 Wed 15:45 SCH A 215

In situ measurement of plasticity accompanying Hydrogen induced cracking — LEONEL STERMANN, LOÏC VANEL, and ●DÖME TANGUY — Institut Lumière Matière, UMR5306 Université Lyon 1 - CNRS, Université de Lyon 69622 Villeurbanne cedex, France

Single crack propagation is studied in a Hydrogen embrittled aluminum alloy. Hydrogen is introduced in the system by electrochemical reactions in an acid aqueous medium. After Hydrogen charging, tensile tests are performed in air, on notched samples, with a micro-tensile machine. An optical microscope is used to follow single crack initiation and propagation at a high magnification. Digital Image Correlation gives the displacement field on the surface with a spatial resolution of about 1 micron. It enables the determination of the position of the crack tip and the local velocity at a sub-grain scale. The equivalent Von Mises strain is calculated and gives a precise measure of the local plastic field which accompanies crack propagation. In addition to the primary plasticity which is emitted from the crack tip or its immediate neighborhood in the form of two intense slip bands, it is systematically found a secondary plastic zone which spreads over several microns ahead of the tip. The characteristics of the plastic zone are measured, together with the velocity and the applied stress intensity factor. In addition, different fracture mechanisms are found on the fracture surface. In particular there are transitions in the fracture mode from intergranular smooth to transgranular parallel to the grain boundary plane. The local fracture mechanisms, in the vicinity of the surface, are linked to the local velocities and plastic deformations.

MM 33.2 Wed 16:00 SCH A 215

Liquid metal induced fracture : modelling and supporting experiments — THIERRY AUGER¹, ANTOINE CLEMENT¹, MARCO EZEQUIEL², ●EVA HÉRIPRÉ¹, INGRID SERRE², ZEHOUA HAMOUCHE¹, JULIE BOURGON³, ERIC LEROY³, and MAXIME VALLET⁴ — ¹PIMM/Arts et Métiers Technology Institute, CNRS, CNAM, 151 Bd de l'hôpital 75013 Paris, France — ²Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France — ³ICMPE - UMR 7182 2/8, rue Henri Dunant 94320 Thiais, France — ⁴MSSMAT, CentraleSupélec, Université Paris-Saclay, France

Liquid metal embrittlement of an otherwise ductile material is an environmentally induced fracture phenomenon characterized by potentially high brittle crack propagation rate and deleterious effects on mechanical properties. Its phenomenology is still not well understood, in particular in terms of prediction of sensible couples and about the detailed intergranular fracture mechanisms. Here we will report on the study in the copper systems via both an energetic and QM/MM approaches at the atomic level to predict the sensitivity of model materials to liquid metal embrittlement. The main goal is to try to link micro-testing (flexion in FIB prepared samples or by in-situ TEM) to a sound modelling at the atomistic scale via fracture mechanics type solicitations. The progress towards predictability of liquid metal embrittlement systems and understanding of fracture mechanisms will be presented along with a vision about their experimental validation.

MM 33.3 Wed 16:15 SCH A 215

Microscale fracture behavior of Laves phases in the Mg-Ca-Al ternary alloy system — ●ANWESHA KANJILAL, UZAIR REHMAN, JAMES P. BEST, and GERHARD DEHM — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Brittle intermetallic Laves phases often act as preferential sites for defects such as cracks in the Mg-Ca-Al alloys. This study investigates the nano- and microscale fracture behavior of C15 Al₂Ca and C14 Mg₂Ca Laves phases prepared as single-phase specimens. Spherical nanoindentation was performed at room temperature in grains of varying surface orientation to identify cleavage planes and orientation effects. Post mortem microscopic examination using electron channeling contrast imaging revealed cracks around indents in both Laves phases, and together with electron backscatter diffraction low index crack planes were identified using trace analyses. For C15 phase, further microcantilever bending and micropillar splitting geometries were fabricated using focused ion beam methodology, wherein fracture toughness $K_{IC} \sim 1.2$ MPa $\sqrt{m}^{0.5}$ was obtained from in-situ testing. Fast screening methodology based on in-situ scratch and nanoindentation at temperatures

from 25 to 500 °C was employed to determine brittle-to-ductile transitions in the Laves phases. The morphology of slip lines and cracks, and decrease in hardness during nanoindentation suggests probable transition $\sim 0.5T_m$ for C15 phase, while studies on C14 are ongoing.

The authors gratefully acknowledge the financial support of Deutsche Forschungsgemeinschaft (DFG) within project B06 of Collaborative Research Center (SFB) 1394, project number 409476157.

MM 33.4 Wed 16:30 SCH A 215

Fracture mechanics concepts in application to functionally graded coatings (FGCs) and FGC structures — ●VERA PETROVA and SIEGFRIED SCHMAUDER — IMWF, University of Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany

The problem of thermal fracture of functionally graded thermal barrier coatings on a homogeneous substrate under the influence of thermo-mechanical loadings is analyzed. It is assumed that FGCs contain a pre-existing system of multiple cracks, edge and/or internal. The thermal and mechanical properties, as well as the fracture toughness of the FGC, are modeled by functions based on the rule of mixtures with a power-law coefficient as the gradation parameter. The problem is formulated using the method of singular integral equation, which are solved numerically. The following fracture characteristics are calculated: stress intensity factors, energy release rates, critical stresses and fracture angles. A series of computational experiments is carried out for FGC/homogeneous structures with typical systems of multiple cracks in the FGC at different gradation parameters and for different material combinations. It is known that the fracture resistance of a TBC can be increased by introducing dense vertical cracks in ceramic coatings; this mechanism is due to the shielding effect in these crack systems. These crack systems are studied and discussed. The goal of this study and the investigation based on the model is to find ways to improve the fracture resistance of FGC/homogeneous structures by avoiding certain critical crack systems.

MM 33.5 Wed 16:45 SCH A 215

Nonlinear elastic effect on interacting crack paths in PDMS films — ●LOIC VANEL¹, OSVANNY RAMOS¹, THIERRY BIBEN¹, STÉPHANE SANTUCCI², and ANTHONY GRAVOUIL³ — ¹ILM - UCBL, Villeurbanne, France — ²LPENS - ENS Lyon, France — ³LAMCOS, INSA Lyon, France

The observed repulsive behaviour of two initially collinear cracks growing towards each other and leading to a hook-shaped path questioned recently the validity of the Principle of Local Symmetry within Linear Elastic Fracture Mechanics theory [1]. Theoretical and numerical work has solved this dilemma, providing the precise geometric conditions for the existence of the repulsive phase and revealing a multi-scale behaviour of the repulsive/attractive transition [2].

Nonlinear elastic materials such as elastomers depart from the prediction of linear elasticity for interacting cracks. We performed experiments on PDMS film that indeed show a maximum angle of repulsion not only significantly smaller than the one of linear elasticity, but also smaller than the one observed in polymer films with a plastic process zone. Our FEM simulations on a Mooney-Rivlin material confirm that the nonlinear elastic response of PDMS modifies the crack path, reducing the repulsive strength between the two interacting cracks.

References [1] Dalbe, M.-J.; Koivisto, J.; Vanel, L.; Miksic, A.; Ramos, O.; Alava, M.; Santucci, S.; Phys. Rev. Lett. 2015 114, 205501 [2] Schwaab, M.-E.; Santucci, S.; Biben, T.; Gravoil, A.; Vanel, L.; Phys. Rev. Lett. 2018 120, 255501.

15 min. break

MM 33.6 Wed 17:15 SCH A 215

Modelling mechanochemical reactions in epoxy resins under tensile load using hybrid QM/MM/MD approaches — ●CHRISTIAN R. WICK¹, MATTIA LIVRAGHI¹, SAMPANNAH PAHI¹, BARISCAN ERICAN¹, DAVID M. SMITH², and ANA-SUNČANA SMITH¹ — ¹FAU Erlangen-Nürnberg, PULS Group, Institute for theoretical physics, Erlangen, Germany — ²Division of Physical Chemistry, IRB, Zagreb, Croatia

Epoxy resins are important thermosetting polymers in our everyday life with a large variety of applications, e.g. as structural materials in

airplanes, as coatings, flooring materials or adhesives. With the aim to understand these complex materials at the molecular scale, we investigate the formation and the mechanochemical response of epoxy resins, including the reactions taking place during curing and under tensile load, by means of quantum chemistry and hybrid Molecular Dynamics (MD) simulations. We present a block chemistry based AMBER force field,^[1,2] which allows generation of fragment partial charges covering all states of curing and fracture, due to cleavage of molecular bonds. Further, we develop an on-the-fly hybrid QM/MM/MD Ansatz to identify bond rupture events in bulk epoxies to improve our understanding of the mechanochemical behavior of these materials.

[1] M. Livraghi, S. Pahi, P. Nowakowski, D.M. Smith, C.R. Wick, A.-S. Smith, Block Chemistry for Accurate Modeling of Epoxy Resins, chemrxiv, 2022 [2] M. Livraghi, K. Höllring, C.R. Wick, D.M. Smith, A.-S. Smith, J. Chem. Theory Comput. 17 (2021) 6449

MM 33.7 Wed 17:30 SCH A 215

Machine Learning of fracture in glasses — FRANCESCO FONT-CLOS¹, MARCO ZANCHI¹, STEFAN HIEMER², ●SILVIA BONFANTI³, ROBERTO GUERRA¹, MICHAEL ZAISER², and STEFANO ZAPPERI^{1,4} — ¹Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy. — ²Institute of Materials Simulation, Department of Materials Science Science and Engineering, Friedrich-Alexander-University Erlangen-Nuremberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — ³NOMATEN Centre of Excellence, National Center for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland — ⁴CNR Consiglio Nazionale delle Ricerche, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia Via R. Cozzi 53, 20125 Milan, Italy.

Being able to predict the failure of materials based on structural information is a fundamental issue with enormous practical and industrial relevance for the monitoring of devices and components. Thanks to

recent advances in deep learning, accurate fracture predictions are becoming possible even for strongly disordered solids, but the sheer number of parameters used in the process renders a physical interpretation of the results impossible. Here we address this issue and use machine learning methods to predict the failure of simulated two-dimensional silica glasses from their initial undeformed structure. We show that our predictions can be transferred to samples with different shapes or sizes than those used in training, as well as to experimental images.

MM 33.8 Wed 17:45 SCH A 215

Using deep neural networks to bridge the gap between statistical fractographic analysis and fracture toughness prediction for polymers — ●GUILLAUME DE LUCA^{1,2}, MOHAMMED IDRI², and LAURENT PONSON^{1,2} — ¹Institut Jean le Rond d'Alembert, Sorbonne Université, CNRS, 4 place Jussieu 75006 Paris, France — ²Tortoise, 231 rue Saint-Honoré, 75001 Paris, France

We propose to deploy DNNs to bridge the gap between statistical fractography and the toughness K_{Ic} prediction for polymers as well as shed light on the role played by the different structures on their fracture surfaces. We generate the fracture surfaces in laboratory through tensile fracture tests while using DIC (Digital Image Correlation) to locally measure and compute the sought mechanical properties along the crack. An interferometric profilometer extracts the topography from the fracture surfaces, and the resulting height fields are post-treated with tools from statistical fractography to be used as input, while the experimental data are used as labels for the regression problem.

By doing so, we can estimate from a scanned fracture surface a material toughness value $K_{Ic}(x)$ along the crack propagation direction. Furthermore, the advancements in explainable neural networks allow us to go one step further by making assumptions about what roughness elements present on the fracture surface influence the most the results coming out of the pipeline.

MM 34: Members' Assembly

Welcome to this general meeting of the DPG-SKM division MM! All of you, presenters of MM talks or posters and other interested participants of this conference, are cordially invited to this meeting. The poster prizes will be presented, here. We will come together in a relaxed atmosphere and exchange information regarding MM. The current conference will be discussed and your feedback will be welcome. We will ask for your suggestions for topics for symposia or speakers to be invited for the next conference. Pretzels and drinks will be provided for free. Take this opportunity to tell us your ideas for MM at the next spring meeting and come to this general meeting of MM.

Time: Wednesday 18:45–19:45

Location: SCH A 251

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

MM 35: Invited Talk: Champion

Time: Thursday 9:30–10:00

Location: SCH A 251

Topical Talk MM 35.1 Thu 9:30 SCH A 251
Configuration entropy and sample size effect on glass transition temperature — ●YANNICK CHAMPION — Univ. Grenoble Alpes, CNRS, Grenoble-INP, SIMaP, 38000 Grenoble, France.

Amorphous materials show an intriguing transition at room temperature between localized and homogeneous deformation. This effect is observed for sample sizes in the micron range for silica glass, tens to hundreds of nm for metallic glasses and less than 20 nm for polymers. It is interpreted as a dependence of the glass transition temperature (T_g) with the sample size. Besides, this has been observed for polymer films and described by an empirical law proposed by Keddie and

collaborators (Keddie et al, Europhys. Lett 1994). A demonstration of this law is proposed from a statistical physics approach and using the potential energy landscape (PEL) description. The work is performed on a Mg-based metallic glass. A configuration entropy is derived from the size distribution of local areas in the PEL favorable to rearrangement. These zones are probed by nano-indentation and assumed to be related to the serrations observed in the deformation curves. The size of the serrations follows a Poisson distribution, indicating that their formation is a rare event. In addition to understanding the effect of size on T_g , the analysis allows the identification of statistical parameters describing the glass structure.

MM 36: Data Driven Materials Science: Big Data and Work Flows – Microstructure-Property-Relationships (joint session MM/ CPP)

Time: Thursday 10:15–13:15

Location: SCH A 251

MM 36.1 Thu 10:15 SCH A 251

Orisodata: A methodology for grain segmentation in atomistic simulations using orientation based iterative self-organizing data analysis — ●ARUN PRAKASH — Micro-Mechanics and Multiscale Materials Modeling (M5), TU Bergakademie Freiberg

Atomistic simulations of the molecular statics/dynamics kind have established themselves as a cornerstone in the field of computational materials science. Large scale simulations with tens to hundreds of millions of atoms are regularly used to study the behavior of nano-(poly)crystalline materials. Identifying grains a posteriori in such simulations is a challenging task, particularly for simulations at high temperatures or at large strains. In this work, we propose a methodology for grain segmentation of atomistic configurations using unsupervised machine learning [1]. The proposed algorithm, called OrISODATA, is based on the iterative self-organizing data analysis technique and is modified to work in the orientation space. The algorithm is demonstrated on a 122 grain nanocrystalline thin film sample in both undeformed and deformed states. The Orisodata algorithm is also compared with two other grain segmentation algorithms available in open-source visualization tool Ovito. The results show that the Orisodata algorithm is able to correctly identify deformation twins as well as regions separated by low angle grain boundaries. The intuitive model parameters relate to similar thresholds in experiments, which helps obtain optimal values and facilitates easy interpretation of results.

References: [1]: M. Vimal, S. Sandfeld and A. Prakash [2022]: *Materialia*, 21, 101314

MM 36.2 Thu 10:30 SCH A 251

Comparison of atomic environment descriptors with domain knowledge of the interatomic bond — ●MARIANO FORTI, RALF DRAUTZ, and THOMAS HAMMERSCHMIDT — ICAMS, Ruhr Universität Bochum, Universität Straße 150, 44801 Bochum

The study of the relative stability of multicomponent materials and the search for new materials for high performance applications requires extensive samplings of the composition space. This is a demanding task due to the computational effort that is required for the electronic structure calculations. In this work we propose a machine learning approach with descriptors of the local atomic environment using different chemistry heuristics based on smooth overlap of atomic positions, recursive solutions of tight-binding Hamiltonians and atomic cluster expansions. We demonstrate that these descriptors, which retain different levels of domain knowledge of structural and electronic properties of the chemical compounds, can be used to predict formation energies with high accuracy even with simple regression algorithms. We apply the methodology to complex crystal structures in binary and ternary intermetallic systems.

MM 36.3 Thu 10:45 SCH A 251

A Machine-Learning Framework to Identify Equivalent Atoms at Real Crystalline Surfaces — ●KING CHUN LAI, SEBASTIAN MATERA, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Functional surfaces and interfaces even of crystalline materials are characterized by breaks of symmetry and long-range order. Yet, even though such a crystalline surface may for instance exhibit numerous vacancies, adatoms, steps, kinks or islands, there are generally still many equivalent atoms, where equivalence refers to an identical or near-identical local environment. There are many equivalent terrace atoms, adatoms, step or kink atoms. In atomic-scale modeling and simulation, identifying these groups of equivalent atoms is a routine task, not least because one would e.g. restrict demanding first-principles calculations like the determination of an adsorption configuration and concomitant adsorption energy to only one site of each equivalence group. Aiming to automatize this routine task, we here present a machine-learning framework to identify all groups of equivalent atoms for any surface or nanoparticle geometry. The initial classification rests on the representation of the local atomic environment through a high-dimensional smooth overlap of atomic positions (SOAP) vector. We then achieve a fuzzy classification by mean-shift clustering within a low-dimensional embedded representation of the SOAP points as obtained by multidimensional scaling (MDS). The performance of this

classification framework will be demonstrated with examples of Pd surfaces.

MM 36.4 Thu 11:00 SCH A 251

Identifying ordered domains in atom probe tomography using machine learning — ●ALAUKEIK SAXENA, NAVYANTH KUSAMPUDI, SHYAM KATNAGALLU, BAPTISTE GAULT, DIERK RAABE, and CHRISTOPH FREYSOLDT — 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. The spatial resolution of APT is $\sim 1\text{-}3$ Å in depth and $\sim 3\text{-}5$ Å in the lateral direction, respectively. Due to the limited spatial resolution, most of the APT data analysis focuses on composition to extract various microstructural features. Here, we aim at identifying additional on-lattice short-range order within an Al-Mg-Li alloy even though the underlying FCC lattice itself is not resolved. We propose a machine learning (ML) methodology to distinguish disordered solid solutions from ordered L12 domains. To encapsulate the local chemistry and noisy structure in APT independent of orientation, we use Smooth Overlap of Atomic Positions (SOAP). To find suitable hyperparameters of the high-dimensional SOAP features, we visualize the data distribution within the latent space of an auto-encoder neural network trained on experimental data with a preliminary classification. After the optimization, synthetic data corresponding to FCC and L12 structures is created with APT level spatial noise and then used for training from scratch a dense neural network for order/disorder classification. The trained model is then able to distinguish between ordered and disordered structures in experimental data.

MM 36.5 Thu 11:15 SCH A 251

Atomic cluster expansion: training a transferable water interatomic potential from the local atomic environments of ice — ●ESLAM IBRAHIM, YURY LYSOGORSKIY, MATOUS MROVEC, and RALF DRAUTZ — ICAMS, Ruhr Universität Bochum, 44780 Bochum, Germany

We show the predictive power of the atomic cluster expansion (ACE) for modeling challenging systems such as water. We trained ACE on data from ab-initio molecular dynamics simulations (AIMD) of water at 300 K. ACE displays excellent agreement to the first-principles reference data in predicting radial distribution functions and covalent and hydrogen bonding characteristics. However, our investigation confirms that describing properties that require sampling a larger fraction of phase space, for example, self-diffusion or the free energies, requires longer AIMD simulation times at different pressures/densities and temperatures. We then show that ice structures provide a more efficient means of sampling the phase space of water: training ACE to diverse ice phases only describes liquid water in quantitative and qualitative agreement with first principles reference data. This reveals a powerful and efficient strategy for building transferable water interatomic potentials without running expensive AIMD.

15 min. break

MM 36.6 Thu 11:45 SCH A 251

Enhancing molecular dynamics simulations of water in comparison to neutron scattering data with algorithms — ●VERONIKA REICH¹, LUIS CARLOS PARDO², MARTIN MÜLLER³, and SEBASTIAN BUSCH¹ — ¹GEMS at Maier-Leibnitz Zentrum, Helmholtz-Zentrum hereon, 85748 Garching, Germany — ²Departament de Física Escola d'Enginyeria de Barcelona Est Universitat Politècnica de Catalunya, 08019 Barcelona, Spain — ³Helmholtz-Zentrum hereon, 21502 Geesthacht, Germany

The structure and dynamics of materials can be studied on the atomic level with neutron and X-ray scattering experiments as well as molecular dynamics (MD) simulations. We connect experimental data with MD simulations to further enhance the simulations and obtain force-fields that are able to reproduce the measured structure and dynamics.

On the example of water, we established a workflow of running MD simulations in the program LAMMPS, calculating X-ray and neutron scattering data with the program Sassena, and comparing the diffrac-

tograms and incoherent intermediate scattering functions to already published experimental data.

The agreement between computed scattering curves and experimental data was optimized with algorithms to obtain a set of parameters that can simultaneously reproduce the real nanoscopic structure and dynamics of water probed by the neutron and X-ray scattering experiments.

This scheme is highly adaptable to different MD simulations of various models.

MM 36.7 Thu 12:00 SCH A 251

Stress and Heat Flux via Automatic Differentiation — ●MARCEL F. LANGER^{1,2,3}, FLORIAN KNOOP^{3,4}, J. THORBEN FRANK^{1,2}, CHRISTIAN CARBOGNO³, MATTHIAS SCHEFFLER³, and MATTHIAS RUPP^{3,5} — ¹BIFOLD – Berlin Institute for the Foundations of Learning and Data, Berlin, Germany — ²Machine Learning Group, Technische Universität Berlin, Germany — ³The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society and Humboldt University, Berlin, Germany — ⁴Theoretical Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — ⁵Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg

Computationally efficient approximations of the Born-Oppenheimer potential energy surface can be obtained by parametrising an analytical force field based on a set of reference calculations. Inspired by recent developments in machine learning, such potentials can include equivariant semi-local interactions through message-passing mechanisms and rely on automatic differentiation (AD), overcoming the need for manual derivative implementations or finite-difference schemes. We provide a unified framework for using AD in such state-of-the-art potentials, and discuss how AD can be used to efficiently and simply compute the stress tensor and the heat flux. We validate the framework by predicting thermal conductivity for selected semiconductors and insulators with an equivariant machine learning potential [1].

[1]: J.T. Frank, O.T. Unke, K.-R. Müller, arXiv 2205.14276 (2022).

MM 36.8 Thu 12:15 SCH A 251

Accurate thermodynamic properties of bcc refractories through Direct Upsampling — ●AXEL FORSLUND, JONG HYUN JUNG, PRASHANTH SRINIVASAN, and BLAZEJ GRABOWSKI — Institute for Materials Science, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart

The outstanding high-temperature properties of the bcc refractory elements make them important in many industrial and scientific applications. Accurate thermodynamic data of unary bcc refractories are a requisite, for example, when used as end members for phase diagrams of high entropy alloys. In this work, we have calculated thermodynamic properties of the four bcc refractory elements V, Ta, Mo and W up to the melting point with full DFT accuracy with the newly developed Direct Upsampling method. We present highly converged Gibbs energy surfaces, from which accurate temperature dependence of heat capacity, thermal expansion coefficient and bulk modulus can be derived. We show their convergence with respect to fitting polynomial order and volume-temperature-grid density. Some group trends are observed, related to the electronic densities of states. In our analysis, we also estimate the contribution from thermal vacancies based on a single high-temperature calculation of the vacancy formation free energy. Further, our results are analysed in terms of homologous temperature for the elements of which a theoretical melting point (connected to the specific exchange correlation functional used) is known. The homologous temperature dependence of the calculated properties show a remarkable agreement with experiments.

MM 36.9 Thu 12:30 SCH A 251

Efficient workflow for treating thermal and zero-point contributions to the formation enthalpies of ionic materials — ●RICO FRIEDRICH^{1,2,3}, MARCO ESTERS¹, COREY OSES¹, STUART KI¹, MAXWELL J. BRENNER¹, DAVID HICKS¹, MICHAEL J. MEHL¹, CORMAC TOHER¹, and STEFANO CURTAROLO¹ — ¹Duke University, USA — ²TU Dresden — ³Helmholtz-Zentrum Dresden-Rossendorf

The formation enthalpy, quantifying the enthalpy of a compound with respect to its elemental references, is a key parameter for predicting the thermodynamic stability of materials thus enabling data-driven materials design. Although for instance zero-point vibrational and thermal contributions to the formation enthalpy can be quite substantial reaching absolute values of up to ~ 50 meV/atom for ionic systems such as oxides, they are often neglected in *ab initio* workflows.

Here, we first calculate the thermal and zero-point contributions accurately from a quasi-harmonic Debye model. At room temperature, they largely cancel each other due to the different bond stiffness of compound and references reducing the total vibrational contribution to maximally ~ 20 meV/atom [1]. Moreover, the vibrational contributions can be parametrized within the coordination corrected enthalpies (CCE) method completely eliminating the need to compute these terms explicitly. On this basis, using only 0 K *ab initio* data as input, a workflow can be designed providing access to formation enthalpies at different temperatures from the AFLOW-CCE tool [2].

[1] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).

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

MM 36.10 Thu 12:45 SCH A 251

Microstructure-Property Linkages for Effective Elasticity Tensors by Deep Learning — ●BERNHARD EIDEL — TU Freiberg, M5-Micro Mechanics & Multiscale Materials Modeling, Lampadiusstraße 4, 09599 Freiberg

The objective of the present work is to link random heterogeneous, multiphase materials to their elastic macroscale stiffness by 3D convolutional neural networks (CNNs). In an approach of supervised learning the effective elasticity tensors stem from homogenization simulations.

The proposed CNN model is a universal predictor for its extended generalization abilities overcoming bottlenecks in existing studies. It accounts for a large variety of microstructures, for arbitrary phase fractions, for almost arbitrary elastic moduli of the constituent phases, and it predicts the stiffness for periodic boundary conditions (BCs) along with sharp upper and lower bounds for the case of non-periodic matter. The proposed universal CNN model achieves high accuracy in its predictions. For a real, two-phase diamond/SiC coating material the universal CNN is almost as accurate as a CNN exclusively trained for fixed elastic phase properties of that material. The speedup compared to finite element computations for homogenization is above factor 20 500. The proposed CNN model hence enables fast and accurate stiffness predictions in universal analyses of heterogeneous materials in their linear elastic regime, for details see [1].

[1] B. Eidel: Deep CNNs as universal predictors of elasticity tensors in homogenization, Comput. Methods Appl. Mech. Eng. (2023).

MM 36.11 Thu 13:00 SCH A 251

Influence of doping atoms on twinning in Ni-Mn-Ga alloy: an *ab initio* study — ●PETR ŠESTÁK, MARTIN HEZCKO, and MARTIN ZELENÝ — Brno University of Technology, Brno, Czechia

Magnetic shape memory alloys (MSMAs) are multifunctional materials which - owing to the tight coupling between their magnetic and ferroelastic order - exhibit interesting phenomena, such as giant magnetoresistance, magnetocaloric and elastocaloric effects, and magnetically-induced reorientation (MIR) of martensite. The prototype MSMAs are the Heusler Ni-Mn-Ga based alloys. By combining the large strain and fast response, they may fill the application gap between the shape memory actuators (large strain, slow response) and magnetostrictive/piezo actuators (small strain, fast response). The MSMAs strongly depends on the twinning structure and especially on the twinning stress that is highly dependent on exact alloy composition, as it significantly decreases with increasing content of Mn, which hinders the MIR in Mn-excess alloy.

The recent development in atomistic simulations allows to determine the twinning stress not only from experimental methods but also from theoretical simulations. For example, generalized-planar-fault-energy (GPFE) curves describe the energy pathways associated with twinning as a function of shearing vector. Here, we present results of our calculations to reveal, how doping elements Co, Cu and Fe affects the GPFE curves, and consequently formation and propagation of twins.

MM 37: Topical Session: Defect Phases II

Time: Thursday 10:15–13:00

Location: SCH A 216

Topical Talk

MM 37.1 Thu 10:15 SCH A 216

Structural and chemical atomic complexity of lattice defects – From defect phase diagrams to properties of intermetallics — MARTINA FREUND, XIE ZHUOCHENG, LUKAS BERNERS, PEI LING SUN, STEFANIE SANDLÖBES-HAUT, and SANDRA KORTE-KERZEL — Institut für Metallkunde und Materialphysik, RWTH Aachen University

Two approaches in materials physics have proven immensely successful in alloy design: First, thermodynamic and kinetic descriptions for tailoring and processing alloys to achieve a desired microstructure. Second, crystal defect manipulation to control strength, formability and corrosion resistance. However, to date, the two concepts remain essentially decoupled. A bridge is needed between these powerful approaches to achieve a single conceptual framework. Considering defects and their thermodynamic state holistically as defect phases, provides a future materials design strategy by jointly treating the thermodynamic stability of both, the local crystalline structure and the distribution of elements at defects.

Here, we will report our work on intermetallics, which are complex already in their underlying crystal structure, to reveal active deformation mechanisms and their dependence on both structure and chemical composition.

MM 37.2 Thu 10:45 SCH A 216

The synthesis and studies of unique oxygen structure on silica-aluminate catalysts — LINFENG SU¹, XU CHEN², HUAPING ZHAO¹, ZHIYI LU², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Key Laboratory of Advanced Fuel Cells and Electrolyzers Technology of Zhejiang Province, Ningbo Institute of Materials Technology and Engineering, CAS, Zhejiang, 315201, PR China

To promote the application of silica-aluminate catalysts in catalytic reactions, the unique active oxygen structures on the surface of silica-aluminate were investigated. 4A molecular sieves were prepared with oxygen-rich vacancies of various contents and different chemical environments. Three different types of oxygen vacancies (due to the covalent and coordination bonds of O) on the surface have different mechanisms in catalytic reactions, and the specific structures exhibit the best catalytic activity (87.5% removal rate of pollutants within 6 min in catalytic ozonation). Moreover, silica-aluminate mullite containing abundant neo-oxygen structure (unique bridging oxygen) was successfully prepared at a low preparation temperature. The abundant oxygen structure in silica-aluminate leads to abundant unique bridging oxygen structures with high catalytic activities (81.2% removal rate of pollutants within 15 min under low ozone concentration). The research on the unique oxygen structure of silicate-aluminate provides theoretical guidance for the design and synthesis of catalysts with high catalytic activities for future industrial applications.

MM 37.3 Thu 11:00 SCH A 216

Understanding corrosion phenomena based on surface phase diagrams for Mg alloys in contact with water — JING YANG, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Düsseldorf, Germany

Defect phases formed at alloy surfaces and interfaces govern their chemical and mechanical behavior. Constructing phase diagrams from ab initio modeling provides valuable information for understanding the microscopic mechanisms of surface and interface processes. In this work, we apply this approach to study the aqueous corrosion of magnesium alloyed with Al and Ca, an important structural material for the automotive and aerospace industries. Constructing defect phase diagrams for the passive film formed on the magnesium surface, we analyze how the Al and Ca alloying atoms evolve during the corrosion process and how they impact the corrosion resistance of the magnesium alloy. In particular, we resolve the cause of Al enrichment in the passive film, which has been recently observed in experiment. Based on these examples we discuss how defect phase diagrams can help us to better understand microscopic chemical processes under realistic conditions.

MM 37.4 Thu 11:15 SCH A 216

Ab-initio informed CALPHAD modelling of grain boundaries — TOBIAS SPITALER¹, RISHI BODLOS², DANIEL SCHEIBER², and LORENZ ROMANER¹ — ¹Montanuniversität Leoben, Department Werkstoffwissenschaft, Leoben, Österreich — ²Materials Center Leoben Forschung GmbH, Leoben, Österreich

The CALPHAD method is an important tool in material science to calculate phase diagrams and to predict phase stabilities of complex systems. Based on a model of the Gibbs Free energy of the bulk phases as function of composition, pressure and temperature the thermodynamic equilibrium quantities can be calculated with computer programs. In materials grain boundaries play an important role for mechanical properties and grain growth. Alloying elements often tend to segregate from or to the grain boundary, changing the properties of the grain boundary for example by weakening or strengthening the cohesion or by preventing grain boundary movement, which can lead to stabilisation of a nano-crystalline structure.

We therefore devise a formulation of the grain boundary Gibbs Free energy within the compound energy formalism with the goal to obtain the grain boundary state parameters such as composition and grain boundary area. We use DFT calculations to explore energy configurations of grain boundaries and couple them to thermodynamic models to investigate solute segregation and its impact on the grain boundary energy. With these results we can provide grain boundary phase diagrams and address thermodynamic nanocrystalline stability in metallic alloys.

15 min. break**Topical Talk**

MM 37.5 Thu 11:45 SCH A 216

Density-based Grain Boundary Phase Diagrams — REZA DARVISHI KAMACHALI — Federal Institute for Materials Research and Testing (BAM)

Phase diagrams are the roadmaps of material design yet primarily developed and discussed for defect-free bulk phases. Real microstructures, however, also contain large populations of defects, such as grain boundaries, which show their own distinct phase behavior. Recently, CALPHAD-integrated density-based phase diagrams were proposed for studying segregation and phase evolution in grain boundaries. In this method, the connection to available bulk thermodynamic data allows rapid assessment of grain boundary phase behavior. In this talk, density-based phase diagrams of several binary and ternary alloy systems will be discussed, with direct implications for alloy and microstructure design. The significance and integration of elastic energies to the density-based model will be presented. It will be shown that Cu segregation and segregation transition in Al-Cu and Al-Cu-Mg systems can be explained by the presence of solutes' elastic interactions with grain boundaries.

MM 37.6 Thu 12:15 SCH A 216

Learning chemistry dependence of grain boundary segregation energies — CHRISTOPH DÖSINGER¹, DANIEL SCHEIBER², OLEG PEIL², VSEVOLOD RAZUMOVSKIY², and LORENZ ROMANER¹ — ¹Montanuniversität Leoben, Department of Materials Science, Leoben, Austria — ²Materials Center Leoben Forschung GmbH, Leoben, Austria

The grain-boundary segregation energy (E_{seg}) is the central quantity for describing the process of grain-boundary segregation which influences fracture. Usually, to obtain highly accurate values for E_{seg} , density functional theory is employed, which incurs high computational costs. This makes it impractical to do a thorough study of segregation to multiple grain-boundaries for a range of solutes. To reduce the number of calculations needed for such a complete description, we apply machine learning methods to density functional theory data. By using separate sets of descriptors for the local atomic environment and the solute types, we fit a model based on gaussian process regression. This approach is evaluated on a comprehensive data-set for E_{seg} in tungsten. The tests indicate that the model has the ability to extrapolate to solutes which are not contained in the training data.

MM 37.7 Thu 12:30 SCH A 216

Rationalising the impact of experimental preparation routes

on impurity content in Pd nano-aerogels using ab-initio phase diagrams — ●MIRA TODOROVA, SU-HYUN YOO, POULAMI CHAKRABORTY, TILMANN HICKEL, SE-HO KIM, BAPTISTE GAULT, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf

Recent advances of experimental techniques with atomic resolution enable us to analyze the structure and composition of samples at the sub-nanometer scale, providing information about contamination with impurities and their distribution. Understanding the factors which govern the ingress, amount and distribution of contaminating elements, opens routes to both improving the sample quality and their utilization in targeted design to achieve a desired functionality. Using an ab-initio based thermodynamic approach and surface phase diagrams we unravel the impact of preparation conditions on experimental observations and materials properties. The power and the performance of these ab-initio based thermodynamic concepts will be highlighted using the example of impurity incorporation during wet-synthesis of nano-aerogels, specifically Na and K incorporation into grain boundaries [JACS 144, 987 (2022)] and B into the bulk [Adv. Mater. 2203030 (2022)] of Pd nano-aerogels.

MM 37.8 Thu 12:45 SCH A 216

Influence of stoichiometric change on plasticity in the Ca(Al;Mg)₂ C15-Laves Phase — ●MARTINA FREUND¹, PEI-

LING SUN¹, CARSTEN THOMAS², DEBORAH NEUSS³, MICHAEL FEUERBACHER², MARCUS HANS³, and SANDRA KORTE-KERZEL¹ — ¹Institut für Metallkunde und Materialphysik, RWTH Aachen University — ²Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen und Peter-Grünberg Institut Forschungszentrum Jülich GmbH — ³Materials Chemistry, RWTH Aachen University

Magnesium is a promising material for light weight applications but is strongly limited because of its low room temperature ductility and low creep resistance. By alloying with Al and Ca different Laves phases form, which improve creep strength properties. We did investigations of the stoichiometric C15 Laves phase, finding slip on {111} and {112} planes with the same activation frequency and approximately same CRSS values. The influence of the stoichiometry regarding the plasticity was analysed using a sample with 6at.-% Mg, by nanoindentation tests, APT and TEM. Hardness and indentation modulus values were in the same range for all indented orientations. Comparing this to the stoichiometric one, the hardness has shown a slight increase around 1 GPa. Changes of plasticity were seen by analysing resulting slip lines. Most activated slip planes were the {112} planes, followed by the {110}. APT was done for both, the stoichiometric and the off-stoichiometric, to evaluate the local chemistry on {112} slip planes. Ultimately, we aim to reveal the connection between the local chemical potential and motion of dislocations on different slip planes.

MM 38: Topical Session: Fundamentals of Fracture – Fracture Experiments

Time: Thursday 10:15–11:15

Location: SCH A 215

Topical Talk

MM 38.1 Thu 10:15 SCH A 215

The Fundamental physics of the onset of frictional motion: How does friction start? — ●JAY FINEBERG — The Racah Institute of Physics, The Hebrew University, Jerusalem Israel

Recent experiments have demonstrated that rapid rupture fronts, akin to earthquakes, mediate the transition to frictional motion. Moreover, once these dynamic rupture fronts ("laboratory earthquakes") are created, their singular form, dynamics and arrest are well-described by fracture mechanics. Ruptures, however, need to be created within initially rough frictional interfaces, before they are able to propagate. This is the reason that "static friction coefficients" are not well-defined; frictional ruptures can nucleate for a wide range of applied forces. A critical open question is, therefore, how the nucleation of rupture fronts actually takes place. We experimentally demonstrate that rupture front nucleation is prefaced by slow nucleation fronts. These nucleation fronts, which are self-similar, are not described by our current understanding of fracture mechanics. The nucleation fronts emerge from initially rough frictional interfaces at well-defined stress thresholds, evolve at characteristic velocity and time scales governed by stress levels, and propagate within a frictional interface to form the initial rupture from which fracture mechanics take over. These results are of fundamental importance to questions ranging from earthquake nucleation and prediction to processes governing material failure.

MM 38.2 Thu 10:45 SCH A 215

Macro to micro in fracture - shorter is tougher — ●DOV SHERMAN — School of Mechanical Engineering, Tel-Aviv University, Tel-Aviv, Israel

Fracture of brittle solids is ultimately executed by atomistic-scale, discrete, and ultrafast bond-breaking mechanisms along the crack path. Here, we show new fracture behavior and properties of brittle materials not previously explored. It is based on macroscopic fracture cleavage experiments of brittle single-crystal silicon specimens, including cracks energy-speed relationships, and an atomistic-scale semi-empirical model for bond-breaking mechanisms in form of planer kinks along the (curved) crack front. As a result, we identified that the cleavage energy is not a constant but bounded by the Griffith Barrier

and lattice-trapping barrier. Hence, a brittle material can be envisaged as having a pseudo-R-Curve behavior typical of metallic materials. A new and essential fracture mechanism was identified, which we termed *quasi-propagation*, occurring between initiation and propagation. During this mechanism, the sequence of the bond-breaking mechanisms is varying, causing an increase in the macroscopic cleavage energy. The range of these changes is dictated by the energy release rate and its first derivative following initiation. The evaluated cleavage energy shows that *shorter is tougher* and hence the material is stronger than that predicted by the Griffith theory.

MM 38.3 Thu 11:00 SCH A 215

How hidden 3D structure within crack fronts reveals energy balance — ●MENG WANG and JAY FINEBERG — The Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, 91904, Israel

Griffith's energetic criterion, has been pervasively used to measure material resistance to failure and describe the propagation dynamics of simple cracks. When cracks contain secondary structure, full crack fronts must be considered. Secondary structure within a crack front will increase energy dissipation, and it is not, a priori, clear how its presence affects the crack dynamics and contributes to the fracture energy. Here, we study low-speed crack propagation in hydrogels under tensile loading conditions. Such slow cracks are shown to be bistable; either simple or faceted crack states can be generated under identical loading conditions. The selection of either crack state is determined by the form of the initial seed crack. We find that seed cracks containing a small local mode III component generally leads to a single step that propagates along a crack front. In contrast to simple cracks, faceted cracks can no longer be considered as existing in a quasi-2D system. For both simple and faceted cracks, we simultaneously measure the energy flux and local fracture toughness along the crack fronts over velocities. We find that the concept of energy balance must be generalized for 3D systems; faceted cracks obey energy balance, only when we account for the local dynamic dissipation at each point along the crack front. If the local structure is not properly accounted for, energy balance will appear to fail.

MM 39: Phase Transformations: Simulation and Machine Learning

Time: Thursday 11:45–13:15

Location: SCH A 215

MM 39.1 Thu 11:45 SCH A 215

Simultaneous structural and thermal characterisation of Zr-based bulk metallic glasses via synchrotron X-ray diffraction and fast differential scanning calorimetry — ●STEFAN T. STANKO¹, JÜRGEN E.K. SCHAWÉ^{1,2}, and JÖRG F. LÖFFLER¹ — ¹Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — ²Mettler-Toledo GmbH, Analytical, 8606 Nänikon, Switzerland

Fast differential scanning calorimetry (FDSC) experiments were performed to measure time-temperature-transformation (TTT) diagrams of Zr-based bulk metallic glasses used for additive manufacturing. The alloys were measured in powder and bulk form, and multiple crystallisation events upon cooling were observed in both cases. The fast differential scanning calorimeter was modified to allow its integration into a synchrotron X-ray beamline and thus to characterise *in situ* metastable phase transformations. With the *in situ* setup it was possible to simultaneously investigate the structure of the phases involved and their transformation kinetics. The results were correlated with the oxygen content of the alloys, with the aim of optimising the additive manufacturing process of metallic parts.

MM 39.2 Thu 12:00 SCH A 215

Measurement and simulation of cooling times in pump-probe experiments of phase transitions with latent heat — ●DANIEL KAZENWADEL, NOEL NEATHERY, and PETER BAUM — Universität Konstanz, Konstanz, Germany

Ultrafast pump-probe experiments are often limited by the need to wait for a sample's back reaction to take place between adjacent laser pulses. Here we investigate by experiments and simulations how the sample geometry influences the cooling rate of VO₂, a strongly correlated phase-transition material with substantial latent heat. We measure back reaction times of milliseconds, microseconds and nanoseconds in free-standing thin-films, coated substrates and bulk crystals, respectively. A simple latent heat model reproduces the behavior of all geometries and can therefore be used to predict the speed of the back reaction in other phase-change materials as well.

MM 39.3 Thu 12:15 SCH A 215

Ab initio thermodynamics and atomistic modeling of NiTi SMA with machine learning interatomic potentials — ●PRASHANTH SRINIVASAN and BLAZEJ GRABOWSKI — Institute for Materials Science, University of Stuttgart, Germany

Equiatomic Nickel-Titanium (NiTi) possesses interesting properties such as pseudoelasticity and shape memory effect that arise from a reversible transformation between the austenite (B2) and the martensite phase (B19'). Other competing phases (B19 and B33) make modeling of NiTi challenging. *Ab initio* molecular dynamics (AIMD) calculations have shown that B19' and B2 phases are entropically stabilized (Haskins et. al., 2016), but the calculations were restricted to a single DFT exchange correlational functional (XC). Studying the kinetics of phase transformation using only DFT is also severely expensive.

In this work, we address both challenges. Using a recently developed thermodynamic integration technique (Jung et. al., 2022) aided with machine-learning based moment tensor potentials (MTPs, Shapeev 2016), it is possible to efficiently compute high-temperature thermodynamic phase stability to DFT accuracy. We perform such calculations to analyze three different XCs (GGA, LDA and SCAN). We also perform large-scale molecular dynamics (MD) simulations using the MTPs to study the kinetically-driven phase transformation behavior in each of these cases. Preliminary results show the necessity of having a high *k*-point density in the underlying DFT calculations. When fitted to such a training set, the MTPs predict highly accurate thermodynamic

properties and phase transformation behavior.

MM 39.4 Thu 12:30 SCH A 215

Prediction of quantum paraelectricity and quantum phase transitions using ab initio self-consistent lattice dynamics and machine learning — ●QUINTIN MEIER¹, AMBROISE VAN ROEKEGHEM², and NATALIO MINGO² — ¹Université Grenoble Alpes, CNRS, Institut Neel, 25 Av. des Martyrs, 38042 Grenoble — ²Université Grenoble Alpes, CEA, LITEN, 17 Rue des Martyrs, 38054 Grenoble, France

Anharmonic interactions of the lattice are essential for understanding the temperature-dependent behavior of many materials. Here we present a method combining DFT and the active learning of interatomic potentials to obtain the necessary sets of forces to calculate the temperature dependent force constants using the quantum self-consistent lattice dynamics formalism [1]. A particularly strong anharmonicity has been shown in incipient ferroelectrics like KTaO₃. We show that our method can be used to accurately and efficiently compute the strongly anharmonic low temperature behaviour of the soft mode in quantum paraelectric KTaO₃, and we study its stability range under pressure and uniaxial strain.

[1] Van Roekeghem, A et al, Comp. Phys. Commun, Vol 263 (2021)

MM 39.5 Thu 12:45 SCH A 215

Atomic cluster expansion for modelling of transition metal carbide systems — ●MINAAM QAMAR — ICAMS, Ruhr University Bochum, Bochum, Germany

Atomic cluster expansion (ACE) provides an alternative to classical and machine learning potentials by modelling the local environment of an atom with a mathematically complete descriptor. We present an ACE potential for the Mo-C system, which is parametrized over an exhaustive dataset of important phases and defect structures. The resulting ACE is shown to be accurate with respect to the DFT reference data and computationally efficient which allows us to perform large scale finite temperature applications.

MM 39.6 Thu 13:00 SCH A 215

Structure-mapping workflow for the investigation of solid-solid phase transitions — ●ARTEM SAMTSEVICH, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Solid-solid transformations are common in nature and in the aging of functional materials. It is thus crucial to understand the origin of these complex phenomena at the atomistic level. The involved activated processes can be modeled as transitions between basins on a high-dimensional free energy landscape (FES). Using the harmonic approximation to transition state theory (hTST), one can estimate reaction rate constants from the location of saddle points on the FES. The chain-of-states method optimizes presumed pathways between two structural endpoints towards the minimum energy pathway (MEP), yielding transition state estimates. The generation of the initial pathway requires the mapping of atomic structures onto each other, which can be achieved either by purely geometrical methods (mapping of atomic positions and cells) or by the topology-based method, which maps the graphs of interatomic bonds. Both approaches are complementary to each other and generate a diverse set of mappings.

The combination of mapping algorithms with the chain-of-state method has recently been merged into a generalized workflow. We will present applications to phase transitions in high-energy-density and superhard materials [1,2] as well as catalyst aging.

[1] Wang, Y., Bykov, M., et al., Nat. Chem. 14, (2022).

[2] Kvashnin, A. G., Samtsevich A.I., Jetp Lett. 111, (2020).

MM 40: Mechanical Properties and Alloy Design

Time: Thursday 15:45–18:30

Location: SCH A 251

MM 40.1 Thu 15:45 SCH A 251

First principles validation of barriers in Ni₃Al — ●ADAM FISHER¹, THOMAS HUDSON¹, HUAN WU², TYLER LONDON², and PETER BROMMER¹ — ¹University of Warwick, Coventry, UK — ²TWI Ltd, Cambridge, UK

Precipitates in Nickel-based superalloys form during heat treatment on a time scale inaccessible to direct Molecular Dynamics simulation, but can be studied using kinetic Monte Carlo (KMC). This requires reliable values for the barrier energies separating distinct configurations over the trajectory of the system. In this study, we validate barriers found with the activation relaxation technique nouveau (ARTn) method in a Ni₃Al using a published potential for the atomic interactions against first-principles methods. In a first step, we confirmed that the ARTn barrier energies agree with those determined with the nudged elastic band (NEB) method. As the number of atoms used in those calculations is too great for direct *ab initio* calculations, we then cut the cell size to 255 atoms, thus controlling finite size effects. We then use the plane-wave density functional theory (DFT) code CASTEP and its inbuilt NEB method in the smaller cells. This provides us with a continuous validation chain from first principles to large-scale KMC and allows us to quantify the errors incurred in simulations of precipitate formation and evolution.

MM 40.2 Thu 16:00 SCH A 251

Ab-initio study of partitioning of transition-metal elements in the γ/γ' microstructure of single-crystal 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

The outstanding mechanical properties at high temperatures of Ni- and Co-base superalloys are closely tied to the underlying γ/γ' microstructure. Understanding the preferences of alloying elements for the γ matrix or γ' precipitates helps to develop new alloy compositions. In this work, we investigate the partitioning of the 3d, 4d, and 5d transition metals (TMs) in Ni₃Al and Co₃(Al,W) superalloys. In particular, we determine the preference of the TM elements for the γ or γ' phase by density functional theory calculations. We find clear trends of partitioning across the TM series that are in good agreement with experimental data. Our findings can be rationalized in terms of band filling and atomic size differences by moments analysis from bond order potential theory.

MM 40.3 Thu 16:15 SCH A 251

Towards understanding the yield stress anomaly of Ni₃Al from the energetics of planar defects — ●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 yield stress anomaly of L1₂ intermetallic compounds, especially Ni₃Al, has been investigated for several decades. It is believed that planar defects, e.g., the complex stacking fault and the antiphase boundaries, play an essential role in the dislocation activities during plastic deformation. However, a thorough temperature dependence of the formation energy of these planar defects is still elusive. Facilitated by the state-of-the-art methodology which acquires different thermal mechanisms, especially the magnetic excitations and the full vibrations, the Gibbs energies of the complex stacking fault and the antiphase boundaries of Ni₃Al were calculated within the ab-initio framework up to the melting temperature. The accurate results obtained here are helpful to scrutinize the available experimentally measured data and provide fruitful insights to understand the mechanism behind the yield stress anomaly as well.

MM 40.4 Thu 16:30 SCH A 251

Observation of in-plane oriented Guinier-Preston zones in Al-Cu — ●JOHANNES BERLIN, TOBIAS STEGMÜLLER, and FERDINAND HAIDER — Universität Augsburg, Deutschland

Known for a long time, the first metastable precipitates forming in Al-Cu alloys during natural ageing are the so-called Guinier-Preston zones (GPZ), platelets of Cu on {100} planes of only one atomic layer thickness. With the development of aberration corrected (S)TEMs, direct observation and imaging of these platelets was possible, but with the restriction, that only edge view was possible. Using a Cs-probe corrected scanning transmission electron microscopy with HAADF detector (DF-STEM), a single Cu atom in a Al column results in sufficient contrast to the neighbouring columns. In sufficiently thin samples, planar zones then lead to theoretically forbidden reflections of type {110} in the fourier transformed image, since only half of the columns in the GP zone contain a Cu atom. Thus, fourier filtering of such an image with only these forbidden reflections allows to observe GP Zones in a plan-view. The average size, shape and density of the GP-zones was determined for different aging times, and STEM image simulations using the software package DrProbe support this interpretation.

MM 40.5 Thu 16:45 SCH A 251

Dynamical and structural properties of undercooled Cu-Ti melts — ●LUCAS KREUZER^{1,2}, FAN YANG², THOMAS HANSEN³, ANDREAS MEYER^{2,3}, and WINFRIED PETRY¹ — ¹Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — ²Institute for Material Physics in Space, German Aerospace Center (DLR), Cologne, Germany — ³Institute Laue-Langevin (ILL), Grenoble, France

Cu-Ti alloys feature a large, undercooled liquid region and a high glass-forming ability (GFA) and thus, provide the possibility to obtain two component bulk metallic glasses (BMGs). This unusual behavior could be due to the special properties of the liquid Cu-Ti system: a positive excess volume and a negative enthalpy of mixing. However, the relevant atomic mechanisms responsible for such good GFA are still to be explored. Here we discuss the temperature-dependent dynamical and structural properties of Cu-Ti melts, within a compositional range of 24 to 69 at% Ti. Accurate data about viscosity, density, and atomic structure, the Cu-Ti samples was obtained by using have been processed without any container using the electrostatic levitation technique. We found a non-monotonous trend of the viscosity, with the highest values at intermediate Ti contents. Surprisingly, this dynamical trend is not reflected by the macroscopic packing fraction, meaning a high viscosity does not necessarily correlate with a dense packing. However, on the atomic scale, x-ray and neutron diffraction reveal a denser, local packing and a pronounced chemical short-range order. These short-range interactions can explain the high viscosity, while the macroscopic packing fraction is rather governed by long-range interactions.

15 min. break

MM 40.6 Thu 17:15 SCH A 251

Can we measure twinning stress of a high entropy alloy with micromechanics? — ●CAMILA AGUIAR TEIXEIRA, SUBIN LEE, and CHRISTOPH KIRCHLECHNER — Institute for Applied Materials, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

CoCrFeMnNi and CoCrNi high entropy alloys (HEAs) have attracted attention due to their mechanical properties. Extensive mechanical twinning is mainly responsible for their outstanding mechanical response under cryogenic temperatures, e.g. increase in ductility and tensile strength. However, at room temperature dislocation slip is dominant and twinning only observed in highly deformed samples. Although both HEAs have been broadly studied, there is still a lack of in-depth understanding of twinning mechanism and stresses required for its activation, which is crucial for advanced HEAs design. In this work, we aim to develop protocols to assess the critical resolved shear stress required for twinning by applying in situ micromechanics. Therefore, two points were addressed within the scope of this work: (i) study the transition from full to partial slip using micropillar compression and (ii) observe deformation twinning by shear stress using micro-shear test. Specific grain orientations were chosen through EBSD analyses, for the micropillar single slip orientation with higher Schmid factor for partial slip and for micro-shear [1 1 2] ND and [-1 1 1] TD orientation. Samples were then micromachined by FIB and tested in situ. Post-mortem analysis included SEM imaging, EBSD and (S)TEM to verify if twinning could be observed. The results provided quantitative insights essential for further understanding of the twinning mechanisms.

MM 40.7 Thu 17:30 SCH A 251

Influence of crystal structure on helium-induced tendrill formation in an FeCoCrNiV high-entropy alloy — ●SVENJA LOHMANN¹, RUSSELL GOODALL², GREGOR HLAWACEK¹, RENÉ HÜBNER¹, LE MA², and AMY S. GANDY² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Germany — ²University of Sheffield, UK

High-entropy alloys (HEAs) are a relatively new class of metal alloys composed of several principal elements, usually at (near) equiatomic ratios. Our goal is to understand how such a multicomponent alloy behaves under irradiation. The FeCoCrNiV HEA exhibits both a face-centred cubic (fcc) and a body-centred tetragonal (bct) phase, thus allowing us to specifically study the influence of crystalline structure at very similar chemical composition. We irradiated both phases with a focussed He beam provided by a helium ion microscope (HIM) at temperatures between room temperature and 500°C. The irradiation fluence was varied between 6×10^{17} ions/cm² and 1×10^{20} ions/cm². High-resolution images of the irradiated areas were taken with the same HIM. Selected irradiated areas were additionally studied by TEM in combination with EDXS. Under irradiation, pores start to be generated in the material with pore sizes differing significantly between the two phases. At higher fluences and above a critical temperature, a tendrill structure forms in both phases. We found that the critical temperature depends on the phase and is lower for fcc. TEM images reveal that the tendrills span the whole depth of the irradiated area, and are accompanied by bubbles of various sizes. Scanning TEM-based EDXS of these structures indicates a He-induced change in composition.

MM 40.8 Thu 17:45 SCH A 251

Diffusion and phase stability in a HCP HfScTiZr multicomponent alloy — ●MOHAN MURALIKRISHNA GARLAPATI¹, SANDIPAN SEN¹, XI ZHANG², SANKARAN S³, JULIANA SCHELL^{4,5}, LUKASZ ROGAL⁶, GERHARD WILDE¹, GRABOWSKI B², and SERGIY V. DIVINSKI¹ — ¹Institute of Materials Physics, University of Muenster, Muenster, Germany — ²Institute of Materials Science, University of Stuttgart, Stuttgart, Germany — ³Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Madras, Chennai, India — ⁴European Organization for Nuclear Research (CERN), CH-1211 Geneva, Switzerland — ⁵Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Essen, Germany — ⁶Institute of metallurgy and Materials Science, Polish Academy of Sciences, Krakow, Poland

Phase stability and tracer diffusion in a hexagonal close-packed (HCP) HfScTiZr multicomponent alloy are investigated. The microstructure stability is examined by an in-depth electron microscopy characterization of samples subjected to prolonged heat treatments. It is found that the alloy decomposes into two HCP phases with similar lattice constants. The DFT calculations confirm the possibility of the phase decomposition. The minor and major phases are observed to be enriched with Ti and Sc, respectively. Self-diffusion is measured using the ⁴⁴Ti, ⁴⁶Sc, and ⁸⁹Zr radioactive isotopes. The phase decomposition is found to influence marginally Zr, but significantly Ti and Sc diffusion. The diffusion properties are analyzed in correlation to the microstructure stability and thermodynamic properties of the alloy.

MM 40.9 Thu 18:00 SCH A 251

Solid solution strengthening in single-phase HEAs based on Au-Cu-Ni-Pd-Pt — ●SOPHIE DRESCHER¹, JENS FREUDENBERGER¹, SASCHA SEILS², ALEXANDER KAUFFMANN², and MARTIN HEILMAIER² — ¹Leibniz-IFW Dresden, Helmholtzstr. 20, 01099 Dresden, Germany — ²Karlsruhe Institute of Technology, Institute for Applied Materials, Engelbert-Arnold-Str. 4, 76131 Karlsruhe, Germany

Solid solution strengthening (SSS) is the dominant strengthening mechanism in High entropy alloys (HEAs). In contrast to dilute alloys, SSS of HEAs is yet not well understood. Therefore, it is necessary to develop reliable models to predict their mechanical properties. To verify such models experimental work is needed that illustrates the concentration-dependent solid solution strengthening of different alloys over a large composition range.

The high entropy alloy system Au-Cu-Ni-Pd-Pt is unique as it crystallizes in face-centered cubic crystal structure and is single-phase presumably within the entire concentration range. Hence, it serves a suitable benchmark system to investigate composition-dependent effects on the strength. In this study, it has been examined whether the model of Varvenne [1] is suitable to predict the SSS in this alloy system. The concentrations of individual elements were varied and the strength and hardness were evaluated. The model of Varvenne is misguiding the development of the strength in a large compositional range. However, the results give insights into the impact of different elements on the strength and can help to further enhance the model.

[1] C. Varvenne, et al., Acta Mater. 118 (2016) 164.

MM 40.10 Thu 18:15 SCH A 251

Magnetism in nanocrystalline CoMnFeNiGa high entropy alloys: "from micro and bulk to nano" — ●NATALIA SHKODICH^{1,2}, VARATHARAJA NALLATHAMBI^{1,2}, TATYANA SMOLYAROVA¹, SVEN REICHENBERGER¹, and MICHAEL FARLE¹ — ¹Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany — ²Max-Planck-Institut für Eisenforschung Max-Planck-Straße 1, 40237 Düsseldorf, Germany

We report the successful fabrication of three types of CoMnFeNiGa high entropy alloys: a) nanoparticles, b) nanocrystalline micron-sized powder, and c) nanocrystalline metallic bulk. Homogeneous micron-sized CoMnFeNiGa HEA powders with a nanocrystalline structure and compositional homogeneity were produced by high energy ball milling (HEBM) for 190 min in Ar at 900/1800 rpm. From these powders we synthesized (a) homogeneous nanocrystalline bulk HEAs by spark plasma sintering (SPS) and (b) HEA nanoparticles - by laser fragmentation in liquids (LFL). The XRD, SEM/EDX, and HR TEM results showed that single fcc phase nanosized grains (~10 nm) are obtained after 190 min of HEBM. These partially transform into a bcc one after SPS at 1073K, while the LFL leads to the formation of nanoparticles with two morphologies, that is spheres and platelets with fcc, bcc and hexagonal structures. Fast annealing up to 1000K of HEBM and LFL HEA particles leads to significant structural and composition changes and increases the saturation magnetization M_s (300K) from 35.4 to 96.1 Am²/kg, and from 37.3 to 49.7 Am²/kg, respectively. We acknowledge financial support from DFG (CRC/TRR 270, project S01).

MM 41: Topical Session: Defect Phases III

Time: Thursday 15:45–18:00

Location: SCH A 216

Topical Talk

MM 41.1 Thu 15:45 SCH A 216

Entropy in grain boundary segregation — ●PAVEL LEJCEK — CEITEC, BUT, Brno, Czechia — Institute of Physics, AS CR, Prague Czechia

Experimentally, a linear dependence between the standard entropy and the standard enthalpy of solute segregation at grain boundaries was established which is called *enthalpy-entropy compensation effect*. In this dependence, there exists a region in which the product of temperature and segregation entropy ('entropy term') is larger than the absolute value of the segregation enthalpy, so that the controlling parameter, the Gibbs energy of segregation, is negative. Under this condition the grain boundary segregation is dominated by the entropy, i.e., the phenomenon of the entropy-dominated grain boundary segregation occurs. We show numerous examples of the grain boundaries and solutes in bcc-iron-based alloys exhibiting this phenomenon. In addition, we formulate the idea that a solute can also segregate at the grain boundary (site) that exhibits positive segregation energy/enthalpy (so called *anti-segregation site*) if the entropy term is larger than the segregation enthalpy, so that the Gibbs energy of segregation is negative. In this way, the solute segregation is completely controlled by the entropy term and an entropy-driven grain boundary segregation will exist. We suggest the entropy-driven grain boundary segregation for several model examples in iron-based systems thus serving as indirect evidence of the phenomenon. Finally, the grain boundary configurational entropy is discussed in relation to its volume counterpart and to the segregation variables.

MM 41.2 Thu 16:15 SCH A 216

Impact of precipitation on grain boundary diffusion in microstructure-engineered Ni-Cr-Fe alloy — ●BAIXUE BIAN, MOHAN MURALIKRISHNA GARLAPATI, SHABNAM TAHERINIYA, SANDIPAN SEN, GERHARD WILDE, and SERGIY V. DIVINSKI — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Grain boundary structure-property relationship is studied in a Ni-based Inconel 602CA coarse-grained alloy using a novel correlative tracer diffusion-analytical microscopy approach. Homogenized and intermediate-annealed states are used to engineer the alloy microstructure. Grain boundary diffusion of Ni and Cr is measured in both C- and B-type kinetic regimes. A co-existence of several short-circuit contributions to tracer diffusion is distinguished and correlated to distinct grain boundary precipitation and segregation as revealed by HAADF-STEM combined with EDX measurements. The homogenized state reveals precipitation of Ni-based L12 and Cr23C6 phases which influence significantly diffusion properties. The intermediate annealing promotes a uniform formation of Cr carbides with a minimal/negligible fraction of the L12 phase. The present study demonstrates the correlated structure-kinetic property measurements provide a unique tool to probe the grain boundary precipitation in these industrially used Inconel alloys.

MM 41.3 Thu 16:30 SCH A 216

Orientation relationship and interface inclination in dependence of heat treatment time between Al2Ca and Mg Matrix — ●LUKAS BERNERS¹, ZHUOCHENG XIE¹, MATTIS SEEHAUS¹, SIYUAN ZHANG², and KORTE-KERZEL SANDRA¹ — ¹IMM, RWTH Aachen — ²MPIE, Düsseldorf

Mechanical properties of two phase-alloys are highly dependent on the morphology of the second phase as well as the interface character. Analysis of the orientation-relationship between the magnesium matrix and C15 (Al2Ca) Laves phase precipitate is up to now mainly conducted via TEM analysis. However, where defect phases as thermodynamically stable interface configurations are to be identified, a more statistically significant approach is needed. To this end, we use large scale EBSD to reveal prevalent orientation relationships as well as interface character during the transition from hexagonal C36 phase to cubic C15 phase during heat treatment at 500 °C and thus unravelling a pathway to the thermodynamically stable interface configuration.

MM 41.4 Thu 16:45 SCH A 216

Non-Arrhenius temperature dependence of grain boundary diffusion in additively manufactured high-entropy CoCr-

FeMnNi alloy — ●NURI CHOI¹, MANOEL W. DA SILVA PINTO¹, SABA KHADEMOREZAIAN¹, SANGSUN YANG², JI HUN YU², JAI SUNG LEE³, GERHARD WILDE¹, and SERGIY V. DIVINSKI¹ — ¹Institute of Material Physics, University of Münster, Münster, Germany — ²Center for 3D Printing Materials Research, Korea Institute of Materials Science, Changwon, South Korea — ³Dep. of Mat. Sci. & Chem. Eng., Hanyang University, Ansan, South Korea

Additive manufacturing process induces numerous crystalline defects such as vacancies, dislocations and dislocation networks, non-equilibrium segregation which affect mechanical, kinetic and structural properties of the fabricated materials. Moreover, a non-equilibrium state of grain boundaries has been discovered, too, which is characterized by enhanced rates of grain boundary diffusion at relatively low temperatures [1]. In the present study, grain boundary diffusion of Ni in additively manufactured CoCrFeMnNi high-entropy alloys is measured in an extended temperature interval. A non-monotonous temperature dependence is observed and interpreted in terms of a thermally-activated relaxation of the non-equilibrium state. The grain boundary energy is evaluated from the grain boundary diffusivity data for various heat-treatment conditions and compared to the total energy released during annealing by differential scanning calorimetry. The evolution of microstructure and mechanical properties is discussed, too.

15 min. break

MM 41.5 Thu 17:15 SCH A 216

Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases — ●ZHUOCHENG XIE¹, DIMITRI CHAURAUD², ACHRAF ATILA^{2,3}, ERIK BITZKE^{2,3}, SANDRA KORTE-KERZEL¹, and JULIEN GUÉNOLE^{4,5} — 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 — ³Department of Materials Science and Engineering, Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — ⁴Université de Lorraine, CNRS, Arts et Métiers Paris-Tech, LEM3, 57070 Metz, France — ⁵Labex Damas, Université de Lorraine, 57070 Metz, France

Synchroshear as the dominant basal slip mechanism in Laves phases is accomplished by the glide of synchro-Shockley dislocations. However, the mechanism of synchro-Shockley dislocation motion is still not well understood. In this work, we demonstrate kink propagation as the energetically favorable mechanism for the motion of synchro-Shockley dislocation using atomistic simulations. Vacancy hopping and interstitial shuffling are identified as two key mechanisms of kink propagation. The assistance of vacancy and antisite defects on kink nucleation and propagation are investigated and shown crucial for kink mobility. These findings provide insights into the dependency on temperature and chemical composition of plastic deformation of topologically close-packed phases.

MM 41.6 Thu 17:30 SCH A 216

Defect bulk-boundary correspondence of topological skyrmion phases of matter — ●SHUWEI LIU^{1,2}, LIKUN SHI¹, and ASHLEY M. COOK^{1,2} — ¹Max Planck Institute for the Physics of Complex Systems, — ²Max Planck Institute for Chemical Physics of Solids

Unpaired Majorana zero-modes are central to topological quantum computation schemes as building blocks of topological qubits, and are therefore under intense experimental and theoretical investigation. Their generalizations to parafermions and Fibonacci anyons are also of great interest, in particular for universal quantum computation schemes. In this work, we find a different generalization of Majorana zero-modes in effectively non-interacting systems, which are zero-energy bound states that exhibit a cross structure, two straight and perpendicular lines in the complex plane, composed of the complex number entries of the zero-mode wavefunction on a lattice, rather than a single straight line formed by complex number entries of the wavefunction on a lattice as in the case of an unpaired Majorana zero-mode. These *cross* zero-modes are realized for topological skyrmion phases under certain open boundary conditions when their characteristic momentum-space spin textures trap topological defects. In the

process of characterizing this defect bulk-boundary correspondence, we develop recipes for constructing physically-relevant model Hamiltonians for topological skyrmion phases, efficient methods for computing the skyrmion number, and introduce three-dimensional topological skyrmion phases into the literature.

MM 41.7 Thu 17:45 SCH A 216

Ga Induced Defect Phase Transformations in the $\Sigma 7$ Mg Grain Boundary — ●PRINCE MATHEWS¹, SIYUAN ZHANG¹, CHRISTINA SCHEU¹, TILMANN HICKEL^{1,2}, and JÖRG NEUGEBAUER¹ — ¹Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf — ²Federal Institute for Materials Research and Testing (BAM), D-12489 Berlin, Germany

The design of tailored materials requires to understand not only bulk phases but also the stability of various defect phases. Grain boundaries (GBs) form one class of defects that directly influence the properties

of the material. Therefore, GB phase transformations introduced by alloying can alter mechanical performance. In this work, the $\Sigma 7$ [0001] | 21.78° (sym. plane 12-38) GB in hcp Mg is investigated, for which an A- and a T-type is known. Ab-initio simulations as a function of stress and temperature (using quasi-harmonic approximation) are performed, and show the presence of a phase transformation. Based on the computed Gibbs energies, the defect phase diagram as a function of the Ga chemical potential is determined. To this end, a complete set of Ga configurations at the GB is first screened with an empirical potential, before accurate ab initio calculations are performed for the low-energy configurations. Ga is not only found to trigger a transformation between T and A type, but a systematic transition of the preferred segregation sites is also seen with an increasing number of Ga atoms at the GB. The results qualitatively agree well with experimental results from high-resolution transition electron microscopy (HR-TEM). Physical mechanisms are provided to explain remaining discrepancies.

MM 42: Interface Controlled Properties and Nanomaterials: Nanoporous Materials and Nanolaminates

Time: Thursday 15:45–18:30

Location: SCH A 215

MM 42.1 Thu 15:45 SCH A 215

Nanoporous high entropy alloys – functional nanoscale networks — ●LUKAS LÜHRS¹, FRIEDERIKE IHLE¹, 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

Both, high entropy alloys as well as nanoporous metals have been the subject of considerable interest in recent years. The former topic explores alloys that are composed of multiple major alloying elements yielding countless opportunities for tailor-made material properties, such as outstanding mechanical performance. The latter investigates self-assembled network structures entirely composed of nanoscale elements. Owing to their large surface area to volume ratio, interfaces of nanoporous metals can be manipulated to obtain functional materials that can be used, e.g. as actuators, sensor or structural material with tunable mechanical properties.

In this work we combine both research topics to make monolithic bodies of a nanoporous high entropy alloy (np-HEA) by dealloying, a selective corrosion method, in aqueous media. Structural investigation finds a uniform, bicontinuous network with feature sizes in the range of a few tens of nanometer. Moreover, samples of np-HEA exhibit a single phase microstructure with homogenous elemental distribution. Compression tests on macroscopic samples reveal considerable mechanical strength. In electrolyte, functionality is introduced by electrochemical modulation of the electrode potential which enables the generation of significant actuation strains.

MM 42.2 Thu 16:00 SCH A 215

Microstructure and mechanical behavior of hierarchical nanoporous gold-polypyrrole electrochemical actuators — ●OLGA MATTS and NADIHA MAMEKA — Helmholtz-Zentrum Hereon, Geesthacht, Germany

Dealloyed nanoporous (np) metals have emerged as promising (electro-)chemical actuators that can compete with conventional actuator materials in terms of large actuation stroke, high strain energy density and low operating voltage [1]. Combining np metals with a conducting polymer polypyrrole (PPy) has been found as an effective way to enhance the actuation strain, mechanical strength and stiffness of np metals [2, 3]. Due to the synergistic effect of the two individual components at the nanoscale, such hybrid structures demonstrate enlarged actuation and tunable elastic modulus amplitudes as well as afford fast response times as compared to PPy alone [1].

In this work, we investigate an effect of structural hierarchy on actuation and elastic properties of *hierarchical* (hc) np-Au/PPy hybrids. We study the behavior in aqueous electrolyte under potential control, exploiting the ability of PPy to change its volume under reversible redox reactions. We reveal pronounced variations in the macroscopic length and Young's modulus in response to the voltage-induced volume changes of PPy. We correlate this behavior with PPy fractions in pores and discuss the underlying mechanisms of the observations.

[1] Wittstock et al. (ed.), RCS (2012). [2] Roschning et al., Adv.

Mater. Interfaces (2020). [3] Li et al., Acta Mater., 212 (2021).

MM 42.3 Thu 16:15 SCH A 215

Electrosorption-Induced Actuation in Nanoporous Silicon — ●MANUEL BRINKER and PATRICK HUBER — Institut für Material- und Röntgenphysik, Technische Universität Hamburg, Denickestraße 15, 21073 Hamburg, Deutschland

Porous silicon provides a scaffold structure to study the confinement related effects of soft matter. We investigate the electro-sorption of electrolyte anions and the electrochemical behaviour of nanoporous silicon in acidic electrolytes. The silicon-electrolyte interface acts as a capacitor which allows the accumulation of electrolyte anions in a chemical double layer by an applied voltage, whose characteristics can be measured by cyclic voltammetry. The surface stresses that are caused to the monolithic porous silicon membrane by such an accumulation lead to a macroscopic strain which can be determined in-situ with a laser beam-bending setup. Comparing nanoporous silicon with a planar silicon surface yields insights on the observed electrocapillarity – in particular with respect to the importance of oxide formation and wall roughness on the single-nanopore scale.[1]

[1] Brinker, M., & Huber, P. (2021). Wafer-Scale Electroactive Nanoporous Silicon: Large and Fully Reversible Electrochemo-Mechanical Actuation in Aqueous Electrolytes. *Advanced Materials*, 2105923.

MM 42.4 Thu 16:30 SCH A 215

Structural analysis of hierarchical nanoporous gold — ●LUKAS RIEDEL¹, JÜRGEN MARKMANN^{1,2}, JÖRG WEISSMÜLLER^{2,1}, and SHAN SHI^{3,1} — ¹Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany — ²Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — ³Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Hierarchical nanoporous metals offer the possibility to produce mechanically stable materials with a reduced solid fraction [1], which therefore qualify for lightweight application. Here, hierarchical nanoporous gold is produced from Ag₉₀Au₁₀, following a three-step procedure which consists of first dealloying, coarsening and second dealloying. The ligament size on the upper and the lower hierarchy level can be tuned independently. In addition to scanning electron microscopy (SEM), small- and ultra-small-angle X-ray scattering (SAXS/USAXS) are applied for structural analysis and show consistent results. Descriptive parameters including length scale, specific surface area and pore volume fraction are obtained. From a comparison of the length scale parameters, ligament diameter and mean ligament distance, a conversion factor is yielded. Ultra-small-angle X-ray scattering was found to be suitable for the analysis of structures with a ligament size range of several hundreds of nanometers.

[1] S. Shi, Y. Li, B.-N. Ngo-Dinh, J. Markmann and J. Weissmüller, Scaling behavior of stiffness and strength of hierarchical network nanomaterials, *Science* 371 (6533), 2021.

MM 42.5 Thu 16:45 SCH A 215

Self-detachment of nanoporous thin films — ●GIDEON HENKELMANN¹, DIANA WALDOW¹, MAOWEN LIU^{1,2}, LUKAS LÜHR^{1,2}, YONG LI^{1,2}, 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

Experiment shows thin films of dealloyed nanoporous gold (NPG) spontaneously detaching from massive gold base layers. NPG can also densify near its external surface. This is naturally reproduced by kinetic Monte Carlo (KMC) simulations of dealloying and coarsening and so appears generic for nanoscale network materials evolving by surface diffusion. This talk focuses on how the KMC simulation manages to predict intricate physical phenomena with few and simple assumptions to the kinetics. This contrasts with contemporary popular efforts to fit a multitude of independent energy barriers to quantum mechanical calculations. Simplified kinetics significantly speed up computation, provide clearer understanding of the underlying processes, while still reproducing relevant phenomena. The KMC simulation model is further motivated by thermodynamic principles.

15 min. break

MM 42.6 Thu 17:15 SCH A 215

Wetting and Drying Dynamics in Hierarchically Porous Silicon: An In-Situ X-Ray Microscopy Study — ●STELLA GRIES^{1,2,3}, LAURA GALLARDO DOMÍNGUEZ^{1,2,3}, MARK BUSCH^{1,2,3}, MARIA LISEANSKAIA^{1,2,3}, JUAN SÁNCHEZ CALZADO^{1,2,3}, MATHIS BODERUS^{1,2,3}, SILJA FLENNER⁴, IMKE GREVING⁴, and PATRICK HUBER^{1,2,3} — ¹Institute for Materials and X-Ray Physics, Hamburg University of Technology, Hamburg, Germany — ²Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ³Center for Hybrid Nanostructures CHyN, University of Hamburg, Hamburg, Germany — ⁴Institute of Materials Physics, Helmholtz Zentrum Hereon, Geesthacht, Germany

Hierarchical porosities consist of small, often nano-scaled pores as well as large, macroscopic pores to simultaneously achieve large inner surfaces in combination with optimized mass transport. The investigation of capillary dynamics within optically opaque hierarchically porous membranes necessitates sophisticated microscopy techniques. First hints to unveil the dynamics are obtained from lab-scale experiments, e.g. mass-uptake as a function of time or the mechanical response depending upon wetting and drying in dilatometry. However, these techniques do not spatially resolve on the rising liquid front, which is achieved with transmission X-ray microscopy (TXM). The samples are scanned in radiography (2D) and tomography (3D) to resolve both the static structure and the capillary dynamics. These findings can help to tailor hierarchical porous materials for their designated application and to tune the dynamics depending on the needs.

MM 42.7 Thu 17:30 SCH A 215

Scaling between elasticity and topological genus of nanoporous metals — ●SEOYUN SOHN^{1,2}, CLAUDIA RICHERT¹, SHAN SHI^{3,1}, JÜRGEN MARKMANN^{1,2}, NORBERT HUBER^{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 — ³Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) made by dealloying has emerged as a model material for random networks and specifically for studies of their mechanics. The mechanical behavior of such open-cell foam structures has been expressed by classical Gibson-Ashby relations. They highlight the solid volume fraction as the most obvious descriptor of strength and stiffness. Yet, recent research acknowledges that Young's modulus, Y , of NPG may significantly depend on additional microstructural descriptors, specifically on the scaled topological genus, g , as a measure of the network's connectivity. It represents the number of connections within a representative volume element of the microstructure. Here, we explore the nature of the dependency of Y on g , and we condense the observations into a scaling law that explicitly involves the scaled genus. Our study inspects and assesses the implications of the existing database, from experiment and simulation, and it adds simulation data for random networks with various scaled genera. The results suggest a common scaling that is broadly comparable to experimental

observations.

MM 42.8 Thu 17:45 SCH A 215

An Improved Kernel-Based NMR Cryoporometry Characterization of Mesoporous Solids — ●HENRY R. N. B. ENNINFUL and RUSTEM VALIULLIN — Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstraße 5, 04103, Leipzig, Germany.

NMR cryoporometry is a pore space characterization technique for industrial and natural materials such as catalysts, gas storage materials, cartilage, bones, rocks and many more. While gaining wide use, the fundamental phenomena underlying solid-liquid phase transitions in geometrically disordered porous materials is still not fully understood. This may lead to inaccurate pore size distributions from the NMR cryoporometry technique.

In this work, we have developed a new approach to NMR cryoporometry. Herein, it takes account of cooperativity effects in pores, the existence of a variable non-frozen layer (NFL) thickness between the frozen core and pore wall and the effect of curvature on thermal fluctuations in pores which hitherto are missing in the current approach. In the first place, we compile a family of transition curves characterizing the phase state in pores with different pore sizes, so called kernels. Thereafter, we apply a general framework for predicting phase equilibria in collection of pores. We demonstrate the new approach by first applying it to ordered porous materials such as MCM-41 and SBA-15. Further more, the technique is used to characterize a highly disordered random porous material where we reproduce all states seen in the material. A more accurate pore size distribution (PSD) is, thus, obtained.

MM 42.9 Thu 18:00 SCH A 215

Interface-related defect annihilation in high entropy amorphous/crystalline nanolaminates under ion irradiation — ●QI XU¹, DANIEL SOPU¹, XUDONG YUAN¹, and JÜRGEN ECKERT^{1,2} — ¹Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, Leoben A-8700, Austria — ²Department of Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, Leoben A-8700, Austria

The main challenge of designing nuclear materials that possess a high irradiation resistance is accumulation of point defects-induced structural damage. The interfaces and grain boundaries play a critical role on the defect generation and annihilation in nanostructured materials. In this work, the irradiation-induced microstructure evolution as well as defect production and recovery in metallic glass (MG) / high entropy alloy (HEA) nanolaminates were investigated by molecular dynamics (MD) simulations. The displacement cascades were simulated for the energies of primary knock-on atoms (PKA) at 5, 10 keV and 15 keV. It was found that, there are more displaced atoms in the thermal spike phase for MG/HEA laminate compared with free-standing MG and HEA. In addition, the interface acts as defect sink and accelerates the recombination and annihilation of interstitial in HEA plate, which leads to more residual vacancies in crystalline plate. Moreover, the residual vacancies diffusion induces the generation of dislocation loops in the HEA plate. Furthermore, the interface acts as a transfer medium that accelerates the crystallization of MG plate during irradiation.

MM 42.10 Thu 18:15 SCH A 215

Anode engineering via ultrathin alumina membrane for next-generation stable sodium metal batteries — ●JIAJIA QIU, CHANGFAN XU, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium metal batteries are recognized as one of the most promising candidates for next-generation batteries, owing to their high theoretical specific capacity and energy density. However, a major bottleneck is the mossy or dendritic growth of Na in the repetitive stripping/plating process with an unstable solid electrolyte interphase (SEI), which limits the Coulombic efficiency and even leads to short circuit risks. In this work, ultrathin alumina membrane (UTAM) is first validated as a functional layer to effectively protect the Na anode for Na-metal batteries. By protecting Na metal with UTAM, the mossy or dendritic growth of Na has been suppressed, resulting in uniform electrodeposition. This highly ordered alumina oxide nanostructure improved electrochemical performance significantly and has the potential to be applied to other metal anodes. The novel design of UTAM protected metal Na anode may bring in new opportunities for next-generation high performance Na metal batteries.