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

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Overview of Invited Talks and Sessions

(Lecture halls C 130, C 230, C 243, and C 264; Poster F)

Invited Talks

MM 2.1	Mon	9:30–10:00	C 130	**Defect phases and their line defects in fcc metal grain boundaries** — •Tobias Brink
MM 9.1	Mon	15:00–15:30	C 130	**Materials Informatics - appreciation of data and algorithms** — •Markus Stricker
MM 30.1	Wed	9:30–10:00	C 130	**Scratching the surface: understanding plasticity associated with microscale asperity contacts** — •Anna Kareer
MM 39.1	Wed	15:00–15:30	C 130	**Exploring Creep-Induced Planar Faults: Segregation Dynamics and Defect Phase Transformations in High Performance Alloys** — •Yolita Eggeler
MM 49.1	Thu	9:30–10:00	C 130	**STZ-vortex unit, a step forward in understanding and controlling shear banding in metallic glasses** — •Daniel Sopu
MM 58.1	Thu	15:00–15:30	C 130	**Liquid-Driven Nanoporous Solids** — •Patrick Huber

Invited Talks of the joint Symposium SKM Dissertation Prize 2024 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H 1012	**Nonequilibrium dynamics in constrained quantum many-body systems** — •Johannes Feldmeier
SYSD 1.2	Mon	10:00–10:30	H 1012	**Controlled Manipulation of Magnetic Skyrmions: Generation, Motion and Dynamics** — •Lisa-Marie Kern
SYSD 1.3	Mon	10:30–11:00	H 1012	**Interactions within and between cytoskeletal filaments** — •Charlotta Lorenz
SYSD 1.4	Mon	11:00–11:30	H 1012	**Field theories in nonequilibrium statistical mechanics: from molecules to galaxies** — •Michael te Vrugt
SYSD 1.5	Mon	11:30–12:00	H 1012	**Lightwave control of electrons in graphene** — •Tobias Weitz

Invited Talks of the joint Symposium Synergistic Imaging Techniques: From Spins and Atoms to Ferroic Domains (SYSA)

See SYSA for the full program of the symposium.

SYSA 1.1	Mon	15:00–15:30	H 0105	**Imaging with coherent soft X-rays** — •Bastian Pfau
SYSA 1.2	Mon	15:30–16:00	H 0105	**Exploring ferroelectric domains and domain wall dynamics with quantitative STEM** — •Marta D. Rossell
SYSA 1.3	Mon	16:00–16:30	H 0105	**Scanning Oscillator Piezoresponse Microscopy: new tools to explore domain wall dynamics** — •Neus Domingo, Shiva Raghuraman, Ralph Bulanadi, Patrycja Paruch, Stephen Jesse

SYSA 1.4	Mon	16:45–17:15	H 0105	**Imaging probe nuclei environments using perturbed angular correlation spectroscopy: Examples from multiferroic $BiFeO_3$** — •Doru C. Lupascu, Thien Thanh Dang, Georg Marschick, Marianela Escobar, Astita Dubey, Ian Yap Chang Jie, Juliana Heiniger-Schell
SYSA 1.5	Mon	17:15–17:45	H 0105	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques, Aurore Finco

Sessions

MM 1.1–1.1	Sun	16:00–18:30	H 0104	**Hands-on Tutorial: Creating and Running Automated Workflows for Material Science Simulations (joint session MM/TUT)**
MM 2.1–2.1	Mon	9:30–10:00	C 130	**Invited talk: Tobias Brink**
MM 3.1–3.9	Mon	10:15–13:00	C 130	**Topical Session: Sustainable metallurgy**
MM 4.1–4.10	Mon	10:15–13:00	C 243	**Data Driven Material Science: Big Data and Workflows I**
MM 5.1–5.5	Mon	10:15–11:30	C 264	**Materials for Storage and Conversion of Energy I**
MM 6.1–6.5	Mon	10:15–11:30	C 230	**Interface Controlled Properties, Nanomaterials and Microstructure Design I**
MM 7.1–7.5	Mon	11:45–13:00	C 264	**Materials for Storage and Conversion of Energy II (joint session MM/KFM)**
MM 8.1–8.5	Mon	11:45–13:00	C 230	**Interface Controlled Properties, Nanomaterials and Microstructure Design II**
MM 9.1–9.1	Mon	15:00–15:30	C 130	**Invited Talk: Markus Stricker**
MM 10.1–10.8	Mon	15:45–18:00	C 130	**Topical Session: Hydrogen in Materials: from Storage to Embrittlement I**
MM 11.1–11.8	Mon	15:45–18:00	C 243	**Data Driven Material Science: Big Data and Workflows II**
MM 12.1–12.4	Mon	15:45–16:45	C 264	**Materials for Storage and Conversion of Energy III**
MM 13.1–13.4	Mon	15:45–16:45	C 230	**Phase Transformations I**
MM 14.1–14.5	Mon	16:45–18:00	C 264	**Materials for Storage and Conversion of Energy IV**
MM 15.1–15.5	Mon	16:45–18:00	C 230	**Phase Transformations II**
MM 16.1–16.18	Mon	18:30–20:30	Poster E	**Poster Ia**
MM 17.1–17.21	Mon	18:30–20:30	Poster F	**Poster Ib**
MM 18.1–18.1	Tue	9:30–10:00	C 130	**Topical Talk: Dierk Raabe**
MM 19.1–19.4	Tue	10:15–11:30	C 130	**Topical Session: Hydrogen in Materials: from Storage to Embrittlement II**
MM 20.1–20.10	Tue	10:15–13:00	C 243	**Data Driven Material Science: Big Data and Workflows III**
MM 21.1–21.5	Tue	10:15–11:30	C 264	**Transport in Materials: Diffusion, Conduction of Charge or Heat I**
MM 22.1–22.5	Tue	10:15–11:30	C 230	**Interface Controlled Properties, Nanomaterials and Microstructure Design III**
MM 23.1–23.5	Tue	11:45–13:15	C 130	**Topical Session: Hydrogen in Materials: from Storage to Embrittlement III**
MM 24.1–24.6	Tue	11:45–13:15	C 264	**Transport in Materials: Diffusion, Conduction of Charge or Heat II**
MM 25.1–25.5	Tue	11:45–13:00	C 230	**Interface Controlled Properties, Nanomaterials and Microstructure Design IV**
MM 26.1–26.3	Tue	14:00–14:45	C 130	**Topical Session: Hydrogen in Materials: from Storage to Embrittlement IV**
MM 27.1–27.3	Tue	14:00–14:45	C 243	**Data Driven Material Science: Big Data and Workflows IV**
MM 28.1–28.2	Tue	14:00–14:30	C 230	**Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials I**
MM 29.1–29.38	Tue	17:00–19:00	Poster B	**Poster II**
MM 30.1–30.1	Wed	9:30–10:00	C 130	**Invited Talk: Anna Kareer**
MM 31.1–31.4	Wed	10:15–11:30	C 130	**Topical Session: Hydrogen in Materials: from Storage to Embrittlement V**
MM 32.1–32.5	Wed	10:15–11:30	C 243	**Developement of Calculation Methods I**
MM 33.1–33.5	Wed	10:15–11:30	C 264	**Transport in Materials: Diffusion, Conduction of Charge or Heat III**
MM 34.1–34.5	Wed	10:15–11:30	C 230	**Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials II**

MM 35.1–35.4	Wed	11:45–13:00	C 130	**Topical Session: Hydrogen in Materials: from Storage to Embrittlement VI**
MM 36.1–36.5	Wed	11:45–13:00	C 243	**Liquid and Amorphous Materials I**
MM 37.1–37.4	Wed	11:45–12:45	C 264	**Transport in Materials: Diffusion, Conduction of Charge or Heat IV**
MM 38.1–38.5	Wed	11:45–13:00	C 230	**Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials III (joint session MM/KFM)**
MM 39.1–39.1	Wed	15:00–15:30	C 130	**Invited Talk: Yolita Eggeler**
MM 40.1–40.11	Wed	15:00–19:05	EMH 225	**Focus Session: Battery Materials – Experimental Characterisation and Safety Testing (joint session KFM/MM)**
MM 41.1–41.6	Wed	15:00–17:00	A 053	**Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides I (joint session DS/MM/O)**
MM 42.1–42.8	Wed	15:30–18:00	C 130	**Topical Session: In Situ and Multimodal Microscopy in Materials Physics I (joint session MM/KFM)**
MM 43.1–43.8	Wed	15:45–18:00	C 243	**Data Driven Material Science: Big Data and Workflows V**
MM 44.1–44.8	Wed	15:45–18:00	C 264	**Developement of Calculation Methods II**
MM 45.1–45.5	Wed	15:45–17:00	C 230	**Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials IV**
MM 46.1–46.3	Wed	17:15–18:00	C 230	**Structurally and Chemically Complex Alloys (joint session MM/KFM)**
MM 47.1–47.31	Wed	17:00–19:00	Poster B	**Poster DS (joint session DS/MM/O)**
MM 48	Wed	18:30–21:00	H 0110	**Members' Assembly**
MM 49.1–49.1	Thu	9:30–10:00	C 130	**Invited Talk: Daniel Sopu**
MM 50.1–50.11	Thu	9:30–13:35	EMH 225	**Focus Session: Battery Materials – Ion Transport, Impurity Effects and Modelling (joint session KFM/MM)**
MM 51.1–51.8	Thu	9:30–12:15	A 053	**Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides II (joint session DS/MM/O)**
MM 52.1–52.7	Thu	10:15–12:45	C 130	**Topical Session: In Situ and Multimodal Microscopy in Materials Physics II**
MM 53.1–53.10	Thu	10:15–13:00	C 243	**Data Driven Material Science: Big Data and Workflows VI**
MM 54.1–54.5	Thu	10:15–11:30	C 264	**Materials for Storage and Conversion of Energy V**
MM 55.1–55.6	Thu	10:15–11:45	C 230	**Liquid and Amorphous Materials II**
MM 56.1–56.5	Thu	11:45–13:00	C 264	**Materials for Storage and Conversion of Energy VI (joint session MM/KFM)**
MM 57.1–57.5	Thu	11:45–13:00	C 230	**Phase Transformations III**
MM 58.1–58.1	Thu	15:00–15:30	C 130	**Invited Talk: Patric Huber**
MM 59.1–59.7	Thu	15:00–17:30	A 053	**Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides III (joint session DS/MM/O)**
MM 60.1–60.8	Thu	15:45–18:00	C 130	**Topical Session: In Situ and Multimodal Microscopy in Materials Physics III**
MM 61.1–61.5	Thu	15:30–16:45	C 243	**Liquid and Amorphous Materials III**
MM 62.1–62.9	Thu	15:45–18:00	C 264	**Developement of Calculation Methods III**
MM 63.1–63.5	Thu	15:30–16:45	C 230	**Functional Materials: Performance, Reliability and Degradation**
MM 64.1–64.5	Thu	16:45–18:00	C 243	**Liquid and Amorphous Materials IV**
MM 65.1–65.5	Thu	16:45–18:00	C 230	**Additive Manufacturing: Microstructure Development**

Members' Assembly of the Metal and Material Physics Division

Wednesday 18:45–20:45 H 0110

MM 1: Hands-on Tutorial: Creating and Running Automated Workflows for Material Science Simulations (joint session MM/TUT)

Time: Sunday 16:00–18:30 Location: H 0104

Tutorial MM 1.1 Sun 16:00 H 0104

Hands-on tutorial: Creating and running automated workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin — [3]ICAMS Ruhr-Universität Bochum, 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 require 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 as also highlighted in the NFDI-MatWerk initiative. 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 give a general introduction to using pyiron, with a focus on atomistic simulation tasks, followed by the construction of fully ab initio phase diagrams obtained by the training and validation of ACE-machine learning potentials providing a real-life application example.

MM 2: Invited talk: Tobias Brink

Time: Monday 9:30–10:00 Location: C 130

Invited Talk MM 2.1 Mon 9:30 C 130

Defect phases and their line defects in fcc metal grain boundaries — •Tobias Brink — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries (GBs) are no longer simply regarded as planar defects, but as objects with distinct atomic structures. In analogy to the bulk, interface thermodynamics can describe GB phases, which also have their own defects, i.e., defects of defects. With atomistic simulations and in close collaboration with atomic-resolution scanning transmission electron microscopy, we investigated different GB phases of fcc $\langle 111 \rangle$ tilt GBs [1]. We find more and more that the presence and nature of GB defects leads to interesting and unexpected phenomena: The junctions of faceted GBs usually drive facet growth (at least on the nanoscale) because of their dislocation-like character and consequently high defect energy. We identified a stable nanofaceted GB structure that eliminates this energy cost and only leaves attractive facet junction interactions due to alternating GB excess stresses [2]. Even on flat GBs, disconnections exist as line defects with a Burgers vector. They are responsible for GB plasticity and couple shear stress to GB migration by introducing a GB step. We show how different GB phases lead to different disconnections that can in turn result in opposite migration directions under the same shear load [3]. Finally, a short overview over other examples of GB line defects will be provided.

[1] Brink, et al., Phys. Rev. B **107**, 054103 (2023)
[2] Brink, et al., arXiv:2309.07595 [cond-mat.mtrl-sci]
[3] Pemma et al., arXiv:2305.10275 [cond-mat.mtrl-sci]

MM 3: Topical Session: Sustainable metallurgy

Time: Monday 10:15–13:00 Location: C 130

Topical Talk MM 3.1 Mon 10:15 C 130

Sustainable Green Ceramics: Future and Perspectives — •Jennifer L.M. Rupp — Technische Universität München, Lehrstuhl für Chemie der Festkörperelektrolyte, Lichtenbergstraße 4, 85748 Garch

Next generation of functional ceramics rely on new ways to not only exchange single elements but looking ahead at redefining sustainable synthesis at low energy and CO2 footprint. The ways we have synthesized functional ceramics for energy storage and conversion devices like batteries, fuel cells, electrolysers, and commodities such as gas turbine, construction, medical and other sectors has been very much laid out over the last 50 years to tackle mostly price. However, as climate change progresses and with 25% of our CO2 footprint steming solely from transportation and material making and assembly in steel and ceramic industry, we need to consider what are alternative and new synthesis ways that drastically reduce our needs in material making. Aspects like socio-economic equality on green materials made at lower footprints and also supply chain security are of essence and we as scientist have to step up the game to propose hads on how solid state chemistry, phsyics and synthesis can be altered to meet sustainability goals. Through the talks examples on functional ceramic trends for physics and chemistry application and devices will be selected per material class, and we will exemplify on the show case of Li+ ion batteries current tech trends and how novel solid state chemistry and physics can support to offer alternatives for a new generation of green functional ceramics at work.

MM 3.2 Mon 10:45 C 130

Data-Driven Design of Recycling Processes for Lithium Ion Batteries — •Nima Emami[1], Luis Gomez-Moreno[2], Anna Kemettinen[2], Rodrigo Serna-Guerrero[2], and Milica Todorović[1] — [1]University of Turku, Turku, Finland — [2]Aalto University, Espoo, Finland

Shifting our focus from mining to extracting materials from waste is essential for sustainable and environmental resource management. We combine lithium-ion battery recycling process simulations with data science to redesign the process for optimal materials recovery, prior to experimental validation. Starting with a model process, we altered processing parameters to simulate 10,000 process outcomes and monitored material flow to identify which parameters maximize the recovery of materials mass for graphite and LiNiMnCoO2 (NMC).

The data analysis shows that the first selected design was suboptimal: while up to 91% of graphite mass could be recovered, its purity was lacking at 70%, and NMC average mass recovery was only 6%. Given that no parameter combination could resolve this problem, we modified the processing stages and repeated the simulations with the enhanced process. We now observed the average graphene purity rise to 99%, while a much broader range of NMC mass outputs indicated that recovery of up to 92% of input mass was possible. Data analysis allowed us to determine parameter combinations that simultaneously optimise the recovery of both graphite and NMC. This study demonstrates that data-driven approaches provide new insights into recycling processes and can facilitate systemic optimisation and design.

MM 3.3 Mon 11:00 C 130

On the origin of embrittlement in Mn containing and Zn-coated steels — •Reza Darvishi Kamachali — Federal Institute for Materials Research and Testing (BAM)

Grain boundary embrittlement in medium-Mn steels and liquid metal embrittlement (LME) in Zn-coated high strength steels are among key challenges on the way of safe application of sustainable steels for automotive industry. Using a novel density-based model for grain boundaries, we reveal that the affinity of a grain boundary to attract Mn and Zn atoms result in a segregation transition accompanied by interfacial structural changes. In case of the Zn, the simulations show that the amount of segregation abruptly increases with decreasing temperature, while the Zn content in the alloy, required for triggering the segregation transition, decreases. The results are discussed in the context of CALPHAD-integrated density-based grain boundary phase diagrams.

MM 3.4 Mon 11:15 C 130

Development of an interatomic potential for iron and its oxides for direct reduction applications — •Baptiste Bienvenu[1], Mira Todorova[1], Jörg Neugebauer[1], Matous Mrovec[2], Yury Lysogorskiy[2], Ralf Drautz[2], and Dierk Raabe[1] — [1]Max-Planck-Insitut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, 44780 Bochum, Germany

Atomistic modeling of iron oxides poses many great challenges, due to their combined structural and electronic complexities, down at the level of electronic structure calculations and up to the length and time scales relevant for the study of mechanisms involved, for instance, in the process of their direct reduction. To leverage these limitations in terms of accessible scales, one requires a physically justified interatomic potential with sufficient accuracy to correctly account for the complexity of iron-oxygen systems, which is not yet available in the literature. In this work, we propose a machine-learning potential based on the Atomic Cluster Expansion for modeling the iron-oxygen system, with an explicit account of magnetism. The model is fitted on an extensive density functional theory database encompassing pure iron and the whole range of possible oxygen containing structures. We test the potential on a wide range of properties of iron and its oxides, including defects and relative stability between different crystal structures and magnetic orders, and demonstrate its ability to describe the thermodynamics of systems spanning the whole range of oxygen content and including magnetic degrees of freedom.

15 min. break

MM 3.5 Mon 11:45 C 130

Artificial negative pressure in DFT+U calculations for iron oxides — •Hao Chen, Christoph Freysoldt, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Off-stoichiometric iron oxides play a crucial role in the process of iron ore reduction. The thermal stability and transformation kinetics of relevant iron oxides depend sensitively on magnetic, configurational, and vibrational degrees of freedom and their interplay, but our understanding in this regard is still limited. In addressing this issue, it's imperative to first achieve a precise and reliable description of the iron oxides, in particular their electronic properties and stability. We employ DFT+U, which is an efficient tool for studying strongly correlated systems, to investigate the stability of Hematite (Fe2O3), Magnetite (Fe3O4), and Wüstite (FeO). We find that the Hubbard U parameter and details of how the projection onto the correlated subspace is implemented may modify even basic materials parameters such as the equilibrium volume by several percent, indicating that the actual ad-hoc choices influence the prediction of lattice constants and bond lengths. We analyze in detail the factors that may contribute to and influence this phenomenon, and explore possible solutions to mitigate the dependence of volume on U.

MM 3.6 Mon 12:00 C 130

Multi-technique investigation of Fe-rich intermetallic compounds for more impurity-tolerant Al alloys — •Shikang Feng[1], Yilun Gong[2], Jörg Neugebauer[2], Dierk Raabe[2], Enzo Liotti[1], and Patrick S. Grant[1] — [1]University of Oxford, UK — [2]Max-Planck-Institut für Eisenforschung GmbH, Germany

During Al alloy solidification, Fe impurities precipitate as coarse (up to millimetres), anisotropic Fe-rich intermetallic compounds (IMCs), severely undermining tensile ductility and toughness, hindering Al recycling. Increasing effort is made to understanding the formation and growth of these IMCs, for a better control of their type, morphology, size and distribution for more sustainable, impurity-tolerant Al recycling processes. In this work, we use *in situ* synchrotron X-ray radiography to study systematically the formation and growth kinetics of $Al_{13}Fe_4$ in a model Al-3wt.%Fe alloy, at cooling rates 0.5-20 Ks^{-1}, representative of industrial conditions. These are then combined with post-solidification electron backscattered diffraction, X-ray computed tomography and atomic-resolution scanning transmission electron microscopy to elaborate on the role of twinning in $Al_{13}Fe_4$ formation and growth mechanisms. Finally, we show how we fuse the multi-technique insights to control the size and morphology of otherwise coarse, plate-like $Al_{13}Fe_4$ using twinning-based modification. The role of targeted alloying additions in the modification and their interplay with twin boundaries is rationalised by density functional theory calculations and atomistic simulations. The work paves a potential pathway to designing next-generation, impurity-tolerant recycled Al alloys.

MM 3.7 Mon 12:15 C 130

On the development of Ni-Fe-Cu anodes for sustainable, CO2-free aluminium electrolysis — •Tom Jamieson[1], Ralf Busch[1], Andrei Iasinkskii[2], Jon Magnusson[3], Gudmundur Gunnarsson[4], Peer Decker[5], Roman Duessel[5], and Isabella Gallino[1] — [1]University of Saarland, Saarbruecken, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]IceTec, Reykjavik, Iceland — [4]Arctus Metals Ltd, Reykjavik, Iceland — [5]TRIMET Aluminium SE, Germany

CO2-free aluminium could be produced from renewable energy sources through an electrolytic process by using inert anodes and wetted drained cathodes as a sustainable substitute to the Hall-Héroult process. Primary aluminium production is a worldwide, energy intensive industry with estimates suggesting the contribution to the global tonnage of greenhouse gas emissions is as high as 1%. The use of consumable carbon anodes in the Hall-Héroult process is a significant contributor to greenhouse gas production, with 1.5t of CO2 produced per tonne of aluminium.

Ni-Fe-Cu alloys have emerged as a strong candidate for inert anodes with a study spanning large parts of the composition space currently lacking. Our work aims to undertake a systematic investigation of the key anodic properties (corrosion resistance, cell stability, purity of resultant aluminium) as a function of the alloy composition to determine an optimal composition range for electrolysis cell performance.

MM 3.8 Mon 12:30 C 130

Order-disorder transitions on alloy surfaces: Full Monte Carlo thermodynamic averages versus Calphad inspired analytical models — Jing Yang, •Mira Todorova, and Jörg Neugebauer — Max-Planck-Insitut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Düsseldorf, Germany

In this work, we propose an analytical thermodynamic model to describe the order-disorder transition on the surface of a metal alloy with substitutional defects. We apply this model on the system of Mg surface with Ca substitutions. First, we show the occurrence of a surface phase transition by using Monte Carlo simulations coupled with cluster expansion. Specifically, the system undergoes a transition from a disordered phase at high temperature and Ca-poor conditions to an ordered phase with 1/3 monolayer Ca coverage at low temperature and Ca-rich conditions. Then we show that with an analytical model which assumes Boltzmann distribution of the phase fractions, it is possible to accurately reproduce the critical transition condition. Last, we compare our method to the sublattice model, which is commonly used in the CALPHAD approach to describe solution phases with ordering. The proposed method provides a simplified model for describing order-disorder transition and is potentially applicable also to constructing bulk phase diagrams.

MM 3.9 Mon 12:45 C 130

Segregation behavior in Ni-based superalloys — •Ahmed Abdelkawy, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str.1, 40470 Düsseldorf

Precipitation-hardened nickel-based superalloys are widely used in aerospace and oil and gas industries due to their high strength and corrosion resistance properties that are retained even at elevated temperatures. The exceptional high-temperature strength characteristics are due to the dispersion of intermetallic phases, such as γ' (Ni3(Al, Ti)) and γ'' (Ni3Nb), within the γ (Ni) Matrix. The corrosion resistance is attributed to the presence of Cr, Nb, and Mo as solid solution within the matrix. The interplay between the matrix, the intermetallic phases, and the dispersed solid solution elements may influence the alloys' properties but remains largely unexplored due to the complexity of the multicomponent nature of these systems. In this study, we examine the segregation behavior of the alloying elements into and around the intermetallic phases and its effect on the corrosion-resistant characteristics of the superalloys. Moreover, we systemically study the thermodynamic stability of the various defects and formed interfaces by constructing defect phase diagrams.

MM 4: Data Driven Material Science: Big Data and Workflows I

Time: Monday 10:15–13:00 Location: C 243

MM 4.1 Mon 10:15 C 243

Investigating Structural Descriptors for High-Dimensional Neural Network Potentials — •Moritz R. Schäfer[1,2], Moritz Gubler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department of Physics, University of Basel, Switzerland

High-dimensional neural network potentials (HDNNPs) are a well established technique to efficiently compute energies and forces akin to ab initio standards for conducting extensive molecular dynamics simulations of intricate systems in high dimensions. This method expresses the total energy from environment-specific atomic energy contributions, with the option to incorporate electrostatic interactions utilizing flexible atomic charges. The reliability of both components significantly depends on the accuracy of the structural descriptors used to define the atomic environments. Here, we combine atom-centered symmetry functions with the newly introduced overlap matrix descriptor. Furthermore, we analyze the strengths and weaknesses of each descriptor, providing insights through demonstrations on benchmark systems.

MM 4.2 Mon 10:30 C 243

Universally Accurate or Specifically Inadequate? Stress-Testing General Purpose Machine Learning Interatomic Potentials — •Konstantin Jakob[1], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Insttitut der MPG, Berlin — [2]Universität Bayreuth

Machine learning interatomic potentials (MLIPs) have revolutionized the field of atomistic materials simulation, both due to their remarkable accuracy - when trained adequately - and their computational efficiency compared to established *ab initio* methods. Very recently, several general purpose MLIPs have been reported, which are broadly applicable across the periodic table. These represent a fascinating opportunity for materials discovery, provided that they are robust and transferable. In this context, metastability and polymorphism pose significant challenges, as the underlying training data sets cannot cover the full space of such structures and compositions. In order to stress test current general purpose MLIPs, we evaluate models based on the M3GNet and MACE architectures on a unique set of inorganic, crystalline materials generated by atom substitutions. Validating these two models, we shine light on both successes and drawbacks of using general purpose MLIPs and evaluate the opportunities that further research can hold.

MM 4.3 Mon 10:45 C 243

Pressure-transferable neural network models for density-functional theory — •Timothy Callow[1], Lenz Fiedler[1], Normand Modine[2], and Attila Cangi[1] — [1]Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Untermarkt 20, Görlitz, 02826, Saxony, Germany — [2]Computational Materials and Data Science, Sandia National Laboratories, 1515 Eubank Blvd, Albuquerque, 87123, NM, USA

Density functional theory (DFT) is well-known as the workhorse of electronic structure calculations in materials science and quantum chemistry. However, its applications stretch beyond these traditionally-studied fields, such as to the warm-dense matter (WDM) regime. Under WDM conditions, there are different challenges to consider (compared to ambient conditions) when using DFT. Namely, the electronic structure problem must be solved (i) for large particle numbers, (ii) for a range of temperatures, and (iii) for a range of pressures. Promising solutions were demonstrated for problems (i) and (ii) [1,2] using a recently-developed workflow to machine-learn the local density of states (LDOS) [3]. In this talk, we discuss our progress in developing a solution for problem (iii). This problem presents additional challenges because the LDOS varies quite significantly with changes in the pressure, making it a difficult problem for neural network models.

[1] L Fiedler et al., npj Comput Mater 9, 115 (2023) [2] L Fiedler et al., Phys. Rev. B 108, 125146 (2023) [3] J. A. Ellis et al., Phys. Rev. B 104, 035120 (2021)

MM 4.4 Mon 11:00 C 243

Towards Multi-Fidelity Machine Learning Using Robust Density Functional Tight Binding Models — •Mengnan Cui[1,2], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth, Physical Chemistry V: Theory and Machine Learning

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. Unfortunately, the sparse availability of DFTB parameters across the periodic table is a significant barrier to the use in many cases. To this end, we introduce a systematic workflow for the robust parameterization of DFTB across the periodic table. Specifically, the parameters for most elements are obtained via Bayesian Optimization on a consistent set of real and artificial elemental solids, spanning a wide range of coordination environments. Elements which do not form stable elemental solids are treated separately, using representative binary compounds as reference. In seeking to bridge the gap towards higher-level quantum mechanical theories, the use of the DFTB parameterization in multi-fidelity machine learning is explored.

MM 4.5 Mon 11:15 C 243

Application of Question Answering method to extract information from materials science literature — •Matilda Sipilä[1], Farrokh Mehryary[2], Emil Nuutinen[2], Sampo Pyysalo[2], Filip Ginter[2], and Milica Todorović[1] — [1]Department of Mechanical and Materials Engineering, University of Turku, Turku, Finland — [2]Department of Computing, University of Turku, Turku, Finland

Scientific text is a promising source of data in materials science, and there is ongoing research how to utilise textual data in materials discovery. In addition to the more established approaches like named entity recognition or dictionary based methods, new machine learning tools such as question answering (QA) are becoming available. The advantages of this method are that it is easy to scale and that it does not require manual text labeling or annotating work, but there may be some loss in precision compared to other methods.

We tested the performance of the QA method on the well-known task of information extraction. We extracted bandgap values of halide perovskite materials from scientific literature. Large language models were tuned towards a specific QA task and then used to select the correct answer for the question about materials properties. In comparison to more established methods, the QA method performed well and we were able to extract correct information from text. This information can be used to map the space of materials properties and find promising new materials solutions. The potential in QA method lies in versatility, accessibility and scalability, since it is easy to use even for researchers with no previous knowledge of language technology.

15 min. break

MM 4.6 Mon 11:45 C 243

Transferable interatomic potential of water with the atomic cluster expansion — •Eslam Ibrahim, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, 44780 Bochum, Germany

We present a transferable parameterization of water using the Atomic Cluster Expansion (ACE). Our approach efficiently samples liquid water by employing static calculations of various ice phases. The active learning feature of ACE-based D-optimality algorithm is utilized to select relevant water configurations, circumventing computational challenges associated with ab-initio molecular dynamics (AIMD) simulations. Our results demonstrate that ACE descriptors enable a potential fitted solely on ice structures to provide a very good description of liquid water. The developed potential shows remarkable agreement with first-principles references, accurately capturing structural and dynamic properties of liquid water. This includes pair correlation functions, covalent bonding profiles, hydrogen bonding profiles, diffusion coefficient, and thermodynamic properties like the melting point of water. This work introduces an efficient sampling technique for machine learning potentials in water simulations, along with a transferable interatomic potential that rivals the accuracy of ab-initio references. This advancement enhances our understanding of water's behavior at the atomic level and opens new avenues for studying complex aqueous systems.

MM 4.7 Mon 12:00 C 243

Automatic extraction and analysis of dislocations in atom probe tomography data using skeletonization — •Alaukik Saxena, Baptiste Gault, 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 a near-atomic resolution for a given material. Extracting and analyzing microstructural features in 3D APT data is challenging and time-intensive, given their complex morphology. Here, we introduce a workflow to systematically extract linear microstructural features, particularly dislocations, from the APT data. The workflow extracts isosurface meshes from APT data and, as a preprocessing step, filters them using principal component analysis (PCA) to find geometrically anisotropic microstructural features. Further, a topology analysis concept called skeletonisation is applied to extract the linear graphs or skeletons of each mesh. Since the skeleton encapsulates the underlying geometry of a mesh, it is used to identify and segment linear features or dislocation segments even in very complex microstructures containing, for example, dislocation networks. This enables a robust composition and geometric analysis of dislocations in APT data. Additionally, the workflow integrates crystallographic data from APT to determine dislocation orientation in the crystal coordinate system. Overall, this advanced workflow significantly reduces manual effort and opens new possibilities for high-throughput studies in material science.

MM 4.8 Mon 12:15 C 243

Stable diffusion based microstructure reconstruction and generation — •Yixuan Zhang[1], Teng Long[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, 64287, Darmstadt, Germany — [2]School of Materials Science and Engineering, Shandong University, 250061, Jinan, China

In recent years, the reconstruction and generation of microstructures have become pivotal in understanding and predicting the mechanical and functional properties of materials. This study introduces a novel approach to microstructure reconstruction based on stable diffusion models. Our implementation employs a stable diffusion model to capture the intricate patterns and features inherent in microstructures, which can be adapted to further refine reconstructed the phase and grain orientation of microstructures, ensuring their statistical and morphological fidelity to the original samples. The model is trained using a comprehensive dataset of 500,000 synthetic micrographs, ensuring the model's robustness and versatility across various material classes. Our results demonstrate that our approach outperforms conventional methods in terms of accuracy, speed, and adaptability. The reconstructed microstructures exhibit remarkable similarity to their counterparts, both qualitatively and quantitatively. Furthermore, the generative capabilities of our model pave the way for optimizing novel microstructures, aiding in the design of materials with desired properties.

MM 4.9 Mon 12:30 C 243

Automatic Generation of Atomic Structure Datasets for Machine Learning Potentials: Alloys and Applicatoin to Mg/Al/Ca — •Marvin Poul[1], Liam Huber[2], and Joerg Neugebauer[1] — [1]Max-Planck- Institut für Eisenforschung, Düsseldorf, Germany — [2]Grey Haven Solutions, Victoria, Canada

We extend a recently proposed strategy for automatically generating training data for machine learning interatomic potentials (MLIP) to alloys.[1]

It is based on small periodic structures (around ten atoms) of various concentrations that are sampled from all crystallographic space groups. These structures are minimized and then again randomly perturbed in positions and cell shape around the obtained local minima. This procedure akin to ab initio random structure search yields samples around the relevant parts of phase space without prior knowledge automatically. Only the cell stoichiometry and the magnitude of the random perturbations remain hyperparameters in this approach.

We explore the natural question of how well potentials can extrapolate in the combinatorically large concentration space and test that they accurately describe structures near the convex hull as well as larger super cells of random alloys. Finally we verify the potentials on binary phase diagrams (and defect phase diagrams) in the ternary Mg/Al/Ca system.

This opens the way for automatic parametrization of MLIPs, promising to bring ab initio accuracy to a large number of systems at scale.

[1]: https://doi.org/10.1103/PhysRevB.107.104103

MM 4.10 Mon 12:45 C 243

Physics-informed neural network for predicting the Gibbs free energy — •Clement Paulson[1], Amin Sakic[2], Vedant Dave[3], Elmar Rueckert[3], Ronald Schnitzer[1], and David Holec[1] — [1]CDL KnowDAS, Department of Materials Science, Montanuniversität Leoben, Austria — [2]Department of Materials Science, Montanuniversität Leoben, Austria — [3]CPS Lab, Montanuniversit Leoben, Austria

We employ a physics-informed neural network approach in conjunction with the CALPHAD formalism to determine the Gibbs free energy of alloys. The Gibbs free energy, essential for CALPHAD simulations, is determined by predicting the Redlich-Kister parameter using a composite neural network utilizing novel descriptors derived from the atomic, composition-based, and thermodynamic properties of elements. The composite neural network comprises a low-fidelity network trained on CALPHAD-generated mixing enthalpies and a high-fidelity network trained on experimental mixing enthalpies. These two models are further connected to a physics-informed neural network, which determines the Redlich-Kister parameters. The predicted Redlich-Kister parameters can then be directly implemented into a thermodynamic database file for immediate use with existing CALPHAD software. This approach holds promise for expediting materials development and phase stability determination. Comparative experimental results highlight the accuracy and potential of this deep learning-based method, offering a novel path for forecasting the Gibbs free energy in multicomponent systems and accelerating the development of databases.

MM 5: Materials for Storage and Conversion of Energy I

Time: Monday 10:15–11:30 Location: C 264

MM 5.1 Mon 10:15 C 264

"Watt's Up" with ^{7}Li: Computing NMR Parameters in Battery Materials Using an All-Electron DFT QM/MM approach

— •Federico Civaia[1], Simone S. Köcher[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Institute of Energy and Climate Research (IEK-9), Forschungszentrum Jülich GmbH, Jülich, Germany

Solid-state electrolytes are crucial in lithium-ion battery research, because of the pressing need for safe and durable high-energy storage solutions. Understanding Li-ion dynamics in these materials is essential for developing improved battery materials. Owing to its non-destructive nature and sensitivity to atomic environments, solid-state nuclear magnetic resonance (SS-NMR) spectroscopy has become an invaluable tool for probing diverse Li-ion environments and investigating Li-ion mobility.

In order to facilitate interpretation of experimental Li SS-NMR spectra, we are setting up a new computational reference scale for a wide range of diamagnetic Li compounds. The efficient calculation of NMR parameters such as the electric field gradient tensor is enabled through the use of the linear-scaling *ab initio* all-electron density-functional theory code FermiONs++ [1] and a solid-state embedding method. The latter hybrid QM/MM (quantum mechanics/molecular mechanics) approach is validated against traditional periodic calculations of SS-NMR parameters for ideal reference systems.

[1] J. Kussman *et al.*, J. Chem. Phys. **138**, 134114 (2013); J. Chem. Theory Comput. **11**, 918 (2015).

MM 5.2 Mon 10:30 C 264

Correlated Motion of Li-Ions and Polarons in Disordered LTO

— •Tavinder Singh[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology

Lithium Ion Batteries are of great importance to our daily lives. Yet, especially with a view on the latter, low reliability and energy density of batteries hamper their adoption. This drives the search for new materials exhibiting favourable properties like high transport efficiencies, wider ranges of electrochemical stability, and, at least for the emerging class of all-solid-state batteries-zero strain on ion insertion for anode materials. In this respect, Lithium Titanium Oxide is a potential candidate exhibiting such properties. In the past, we have shown that in this material the electronic conductivity is due to the formation of polarons, which in turn might influence the movement of ions. Yet, a full study of the possibly correlated motion of both types of carriers is still lacking due to the combinatorial explosion of possible polaron and ion sites making it hard to compute necessary energies and barriers from first principles. Thus, we used a compressed sensing model based on Density Functional Theory energetics to increase the efficiency of our sampling and obtain a full description of conductivity and correlated motion in $Li_4Ti_5O_{12}$.

MM 5.3 Mon 10:45 C 264

High-throughput computational screening of fast Li-ion conductors for solid-state electrolytes

— •Tushar Thakur[1], Loris Ercole[1], and Nicola Marzari[1,2] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Paul Scherrer Institut, Villigen, Switzerland

We present a high-throughput computational screening to find fast lithium-ion conductors to identify promising candidate materials for application in solid-state electrolytes. Starting with ~30,000 experimental structures sourced from the COD, ICSD and MPDS repositories, we perform highly automated calculations using AiiDA at the level of density functional theory (DFT) to identify electronic insulators. On these ~1000 structures, we use molecular dynamics (MD) to estimate lithium-ion diffusivities using the pinball model [1], which describes the potential energy landscape of diffusing lithium at near DFT accuracy while being 200-500 times faster. Then, we study the 50 most promising unknown fast conductors with full first-principles MD simulations. We present this entire screening protocol, including the workflows where the accuracy of the pinball model is improved self-consistently, necessary to automatically running the required calculations and analysing their results.

[1] L. Kahle, A. Marcolongo and N. Marzari, Modeling lithium-ion solid-state electrolytes with a pinball model. Phys. Rev. Mater. 2, 65405 (2018)

MM 5.4 Mon 11:00 C 264

Mechanical testing of LiCoO2 battery electrode and effect of de-/lithiation

— •Robert Löser, Yug Joshi, and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart, Deutschland

The mechanical characteristics of lithium-ion cathode materials play a crucial role in determining key battery performance such as durability, cycle life, and safety. This study focuses on LiCoO2 (LCO), a widely used layered-structured cathode material for lithium-ion batteries, and investigates its mechanical properties during delithiation using sputtered thin films and nanoindentation techniques. The research reveals a significant decrease in Young's modulus from 275.9GPa to 243.4GPa upon lithium-ion deintercalation, attributed to alterations in bonding interactions. After subjecting the sample to extensive cycling, the decline in Young's modulus after the delithiation is reduced to 4.3% with a Young's modulus for the fully lithiated state of 255.5GPa. Additionally, this investigation identifies a linear increase in the proportion of elastic deformation with decreasing lithium content. Furthermore, the experiment in comparison to finite element method (FEM) simulations suggest the propagation of a Li0.5CoO2 phase from the top of the layer during delithiation. This work sheds light on the dynamic changes in mechanical properties of LCO, providing valuable insights for the design and optimization of lithium-ion batteries.

MM 5.5 Mon 11:15 C 264

Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials

— •Yuandong Wang, Yute Chan, Kyeonghyeon Nam, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin, Germany

Garnet $Li_7La_3Zr_2O_{12}$ (LLZO) is a highly promising solid electrolyte for lithium batteries. However, its practical application faces challenges, primarily arising from Li dendrite formation and the impact of grain boundaries (GBs) on Li transport and stability. The amorphous LLZO exhibits desirable properties like blocking Li dendrite growth, high Li mobility and high electronic impedance. Control over amorphous domains between crystalline grains promises a method for tuning electrolyte performance. An atomistic understanding of the interplay between composition, structural characteristics and the properties of LLZO glass-ceramics is required for rational electrolyte and GBs design.

Machine Learning Interatomic Potentials (MLIPs) offer an accurate and efficient way to explore complex structures by enabling large-scale molecular dynamics (MD) simulations. In our study, we first establish a baseline MLIP using a dataset containing c-LLZO with varied Li configurations. Then an iterative training protocol employing simulated annealing to gradually produce amorphized GB motifs is utilized. The converged MLIP enable the construction of realistic models for amorphous LLZO and GBs in LLZO electrolytes, paving the way for their detailed exploration.

MM 6: Interface Controlled Properties, Nanomaterials and Microstructure Design I

Time: Monday 10:15–11:30 Location: C 230

MM 6.1 Mon 10:15 C 230

Learning the influence of chemistry on grain-boundary segregation — •Christoph Dösinger[1], Oleg Peil[2], Daniel Scheiber[2], Vsevolod Razumovskiy[2], and Lorenz Romaner[1] — [1]Montanuniversität Leoben, Department of Materials Science, Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Leoben, Austria

The grain-boundary segregation energy is the central quantity for describing the process of grain-boundary segregation which influences interfacial properties. Usually, to obtain highly accurate values for segregation energies, 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 calculation needed for such a complete description, we apply machine learning methods to density functional theory data. In this talk I will show, how one can train machine learning models that cover the periodic table of elements. By combining element specific features and features of the local atomic structure, these models are able to generalize to different elements and grain-boundaries and accurately predict the segregation energies. The method is tested on a comprehensive data-set of segregation energies in W and then applied in an active learning loop for learning segregation in Cr.

MM 6.2 Mon 10:30 C 230

Grain boundary nanofacets stabilized by facet junction interactions in fcc metals — •Tobias Brink, Lena Langenohl, Swetha Pemma, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

If grain boundary (GB) energies are sufficiently anisotropic, GBs can dissociate into facets to reduce their (free) energy. While mostly splitting of asymmetric GBs into symmetric facets is observed, faceting of symmetric GBs into different symmetric GB planes was also reported (mainly for incoherent $\Sigma3$ tilt GBs in fcc). This, in any case, introduces line defects at the facet junctions, which typically present a driving force to grow the facets in order to reduce the total number of junctions and thus the system's energy. Often, facets are micrometer sized and facet growth only arrests for kinetic reasons. So far, energetically stable, finite-sized facets have not been observed, even though theoretical stability conditions have been proposed. Here, we show a case where nanometer-sized facets are indeed stable compared to longer facets in [111] tilt GBs in Cu by atomistic simulation and transmission electron microscopy [1]. This occurs for misorientations that deviate from $\Sigma3$ (60°), such as $\Sigma19b$ (46.8°) and $\Sigma37c$ (50.6°). In constrast to $\Sigma3$, these facet junctions lack a Burgers vector component, which is unusual. Thus, only attractive junction interactions via line forces resulting from the GB excess stress remain, resulting in stable facet lengths of 1–3 nm. Atomistic simulations predict that the same phenomenon also occurs in at least Al and Ag.

[1] Brink, Langenohl, et al., arXiv:2309.07595 [cond-mat.mtrl-sci]

MM 6.3 Mon 10:45 C 230

Segregation of light elements (H, B, C, N, O, P, S) to ferritic iron grain boundaries: A first principles study — •Han Lin Mai[1], Tilmann Hickel[1,2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany

Segregation of alloying or tramp elements to grain boundaries can drastically affect the properties of metallic alloys. Understanding segregation to grain boundaries is an important step towards constructing their defect phase diagrams and therefore critical to enable rational grain boundary engineering for alloys design. Smaller elements such as (H, B, C, N, O, P, S) often play a crucial role in segregation phenomena, but their positioning at grain boundaries are often ambiguous and make them challenging to study. To study the large number of possible 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 thus constructed large ab initio data sets we derive and discuss chemical and structural trends observed in the solute segregation behaviour. The features which are most important in evaluating site segregation for small elements are derived and discussed. We also benchmark various interatomic potentials against our DFT data to assess their compatibility with segregation studies.

MM 6.4 Mon 11:00 C 230

Exploring the links between local interface chemistry and mechanics using in situ micromechanical testing — •James P. Best — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany

The mechanisms governing dislocation plasticity and fracture at the smallest scales is critically linked to chemistry, in particular at defects, in dictating material behaviour. This has been demonstrated using in situ electron microscopy testing of, for example, copper and tungsten containing trace impurities at grain boundaries. For the study of recrystallised tungsten, in situ microcantilever testing coupled with atom probe tomography provided insights into the effects of impurity segregation on the toughness by placing the notch directly at grain boundaries. For both as-received material and single-crystalline recrystallised tungsten, plasticity was accumulated before failure through ductile crack tip tearing. In contrast, the toughness at grain boundaries dropped sharply, regardless of grain boundary misorientation or grain orientation. Atom probe analysis of the grain boundaries showed segregation of phosphorous to the recrystallised interfaces. Atomistic simulations of a model $\Sigma7$ tungsten grain boundary containing phosphorous confirms a significant embrittlement along the decorated boundary. By elucidating such local chemical effects, we aim to pave the way for the design of materials with enhanced strength and toughness.

MM 6.5 Mon 11:15 C 230

Insights into Microstructure Evolution through Continuum Modeling of Disconnection-Mediated Interface Migration — •Marco Salvalaglio[1], Caihao Qiu[2], Jian Han[2], and David Srolovitz[3] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR, China — [3]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China

Interface migration in microstructures is mediated by the motion of line defects with step and dislocation character, i.e., disconnections. We illustrate a continuum model for arbitrarily curved grain boundaries or heterophase interfaces accounting for disconnections' role in the usual phenomenology of microstructure evolution. We discuss recent model advancements and applications. These include accounting for multi-mode disconnections, namely different step heights for disconnections nucleating on a given grain boundary, and phase field modeling. Numerical results are shown to reproduce molecular dynamics simulations. Implications for interface faceting and change in relative orientations of grains are discussed. Refs: Acta Materialia 227, 117178, (2022); Acta Materialia 227, 117463, (2022); Acta Materialia 251, 118880 (2023).

MM 7: Materials for Storage and Conversion of Energy II (joint session MM/KFM)

Time: Monday 11:45–13:00 Location: C 264

MM 7.1 Mon 11:45 C 264

Symmetry Matters: Machine Learning EFG Tensors for NMR Parameter Simulations — •Angela F. Harper[1], Simone Köcher[1,2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]IEK-9 Forschungszentrum Jülich

Electric field gradient (EFG) tensors are directly probed by experimental solid-state Nuclear Magnetic Resonance (NMR), and are crucial for deciphering the atomic-scale structure and dynamics of Li-ion battery materials. By employing a machine learning approach we devise a model capable of learning complete EFG tensors, using equivariant descriptors. We further show that it is not sufficient to simply learn scalar quantities derived from a tensor such as quadrupolar shift or asymmetry. To assess the model's performance, we curate an extensive dataset comprising over 60,000 EFG tensors calculated for a diverse set of equilibrium and non-equilibrium crystal structures of $Li_4Ti_5O_{12}$ (LTO), a well-studied zero-strain insertion anode material in Li-ion batteries. We finally show that we predict the quadrupolar frequency to within a few kHz for the ^{7}Li nucleus, which is well within the level of error required to make meaningful predictions for ^{7}Li NMR. This work represents a significant step towards realizing *in silico* spectroscopy: the ability to calculate spectroscopic signals such as EFG tensors with the same accuracy as experimental spectroscopy, using machine learning.

MM 7.2 Mon 12:00 C 264

Design criteria for zero-strain cathode materials of the tungsten bronze type compounds A_xFeF$_3$ (A=Li, Na, K) by first-principles — •Aljoscha F. Baumann[1], Daniel Mutter[2], Daniel F. Urban[1,2], and Christian Elsässer[1,2] — [1]Freiburg Materials Research Center, 79104 Freiburg, Germany — [2]Fraunhofer IWM, 79108 Freiburg

Mechanical stresses in the microstructure of cathode materials during charge/discharge cycles can reduce the long-term stability of intercalation-type alkali-metal-ion batteries. In this context, crystalline compounds exhibiting *zero-strain* (ZS) behavior are of particular interest. For instance, near zero-strain sodiation was experimentally measured in the tetragonal tungsten-bronze (TTB) type compound Na_xFeF_3. [Han, J. Mater. Chem. A, 4, 7382] By atomistic simulations, using a first-principles method based on density functional theory, we investigated the potential of iron-based fluoride compounds with tungsten-bronze structures as ZS cathode materials. The simulations were conducted systematically to study the intercalation of the alkali metal ions Li^+, Na^+, and K^+ into the TTB and two related tungsten-bronze structures of the perovskite and hexagonal types. As the alkali-metal ions intercalate, the oxidation state of the Fe ions decreases, which leads to an enlargement of their surrounding Fluorine octahedra. We found that this effect can be partially compensated by the volume reduction of the F- polyhedra surrounding the alkali ions. We discuss the structural and chemical prerequisites of the host lattice for enabling a ZS insertion mechanism for ions in crystals.

MM 7.3 Mon 12:15 C 264

Construction of cobalt oxyhydroxide nanosheets with rich oxygen vacancies as high-performance Lithium-ion Battery anodes — •Yonghuan Fu[1,2], Huaping Zhao[1], Jianhong Liu[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Graphene Composite Research Center, College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, P. R. China

Cobalt oxyhydroxide (CoOOH) is a promising anode material for lithium-ion batteries (LIBs) due to its high electronic conductivity and theoretical specific capacity. Herein, CoOOH nanosheets are successfully obtained using a facile one-pot method, and a hierarchical nanoporous structure is formed by oxidizing cobalt hydroxide (Co(OH)2) in NaOH and (NH4)2S2O8 solution. The CoOOH anode shows better electrochemical performance compared to Co(OH)2 and Co3O4 electrodes when applied to LIBs. The hierarchical nanoporous structure and high electronic conductivity of the CoOOH anode contribute to its outstanding initial discharge capacity, high initial coulombic efficiency, and excellent cyclability. Experiments and density functional theory (DFT) calculations confirmed that the high ICE and prominent rate capability of the nanosheets could be ascribed to the rapid and complete conversion reaction of CoOOH upon lithiation/ delithiation facilitated by hydroxyl groups and oxygen vacancies. This study provides new insights into the structure-property relationship of transition-metal oxyhydroxide anode materials for LIBs.

MM 7.4 Mon 12:30 C 264

Preparation of Prussian blue analogue materials and their application to sodium ion storage — •Ping Hong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The development of a new generation of energy storage systems is necessary due to the limited availability of non-renewable energy resources and the substantial environmental impact associated with the utilization of renewable energy. Sodium ion batteries are likely to become the next generation of large-scale commercial energy storage systems because of their low cost and high energy density. Among various materials, Prussian blue analogs (PBAs) have received great attention for their open three-dimensional framework structure and rapid sodium ion insertion/de-insertion capability. And derivatives synthesized using PBAs as templates have been widely studied. Therefore, in this work, PBAs with a well-defined structure were prepared as cost-effective electrode materials by a simple co-precipitation method. The PBAs materials were applied to sodium ion batteries, showing excellent performance. To achieve outstanding performance, a series of adjustments were made to the binder, electrolyte, and voltage range used in the batteries. at a current density of 100 mA g-1 within the voltage range of 2.0-4.2 V, the capacity remains around 120 mAh g-1. Even at ultra-high loadings, the material demonstrates excellent capacity and cycling stability.

MM 7.5 Mon 12:45 C 264

Multiscale defective FeCu interfaces for sodiophilic and catalytic-enhanced Na-CO2 batteries — •Changfan XU, Tzuchin Huang, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium-carbon dioxide (Na-CO2) batteries are hindered by challenges such as unmanageable sodium deposition/ volume changes at anode and sluggish CO2 reduction/ evolution reaction (CO2RR/ CO2ER) kinetics at CO2 cathode upon cycling. Here, we propose a dual-functional electrode with multiscale defective FeCu interfaces (CP@FeCu) that acts as Na metal hosts and CO2 cathode simultaneously. Microstructural, electrochemical reaction, and theoretical calculations investigations collectively reveal that multiscale defective FeCu interfaces are responsible for the enhancement of sodiophilicity for Na plating/stripping at anode and catalytic activity for CO2RR/ CO2ER at CO2 cathode. Consequently, the CP@FeCu anode enables the uniform deposition of dendrite-free sodium, and the CP@FeCu cathode exhibited low overpotentials and exceptional long-term cycling stability. Significantly, implementation of a symmetrical Na-CO2 battery with CP@FeCu@Na anode and CP@FeCu cathode demonstrates significantly improved electrochemical properties. The introduction of multiscale defective FeCu interfaces with sodiophilic and catalytic dual centers offers an effective method for the tailoring and optimization of sodium metal batteries with high energy density.

MM 8: Interface Controlled Properties, Nanomaterials and Microstructure Design II

Time: Monday 11:45–13:00 Location: C 230

MM 8.1 Mon 11:45 C 230

Topology-dependent scaling behavior of stiffness and strength of hierarchical nanoporous metals — •Lukas Riedel[1], Jürgen Markmann[1,2], and Shan Shi[3,1] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Structural hierarchy in nanoporous metals allows optimized functional and mechanical properties in lightweight materials. In this work, hierarchical nanoporous gold with two distinct length scales is synthesized via a dealloying-coarsening-dealloying method. This method enables tuning the structure of the lower and upper hierarchy level independently. The structural parameters including ligament diameter, ligament distance, solid fraction, and topological connectivity are characterized by combining focused ion beam tomography with small- and ultra-small-angle X-ray scattering. The mechanical studies indicate that consistent with the connectivity, the effective macroscopic Young's modulus and the normalized strength also highly depend on the ligament size of both the upper and the lower hierarchy level. These experimental findings serve as basis for the development of a topology-dependent scaling law for the stiffness and strength of random hierarchically nested-network nanomaterials.

MM 8.2 Mon 12:00 C 230

In-situ studies on the formation of nanoporous copper during electrochemical dealloying — •Samuel Graf[1], Eva-Maria Steyskal[1], Elisabeth Hengge[2], Tatiana Kormilina[3], and Roland Würschum[1] — [1]Institute of Materials Physics, NAWI Graz, Graz University of Technology, Austria — [2]Insitute of Biotechnology and Biochemical Engineering, NAWI Graz, Graz University of Technology, Austria — [3]Austrian Centre of Electron Microscopy and Nanoanalysis, Steyrergasse 17, 8010 Graz, Austria

Nanoporous metals formed by dealloying, a selective etching process which removes the less noble component(s) from an alloy, are versatile systems due to their self-similar, free-standing, conductive structure with very high surface-to-volume ratio. The here presented bulk nanoporous copper (np-Cu), produced from Mn-Cu [1] and Al-Cu alloys, represents a highly interesting alternative to the well-known nanoporous gold structure, both from an economic as well as a sustainability persperspective. Insights to the formation process of np-Cu are provided by in-situ resistometry during the electrochemical dealloying process, and supported by ex-situ scanning electron microscopy imaging after dealloying. The results show that compared to more noble metals, the surface reordering during nanoporous structure formation is suppressed on np-Cu. This is assigned to the stronger formation of oxides, which yields interesting properties for possible future applications. Financial support by the FWF project P 36409 is appreciated.
[1] Hengge et al. Nanoscale Advances **5** (2023) 393-404

MM 8.3 Mon 12:15 C 230

In-situ xray nanotomography of the isothermal structural-topological evolution of nanoporous gold — •Markus Ziehmer[1,2], Kate L.M. Elder[3,4], Jürgen Markmann[2], Yijuan Wu[2], Tiberiu Stan[4], Jin Zhang[4], Xianghui Xiao[5], Erica T. Lilleodden[6,2], and Peter W. Voorhees[4] — [1]Universität Ulm, Institut für Funktionelle Nanosysteme, — [2]Helmholtz-Zentrum Hereon, Institut für Werkstoffmechanik — [3]Lawrence Livermore National Laboratory — [4]Northwestern University, Department of Materials Science and Engineering — [5]Brookhaven National Laboratory, National Synchrotron Light Source II — [6]Fraunhofer IMWS, Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen

The structural coarsening of nanoporous gold and other metallic, bicontinuous systems is inherently linked to topological transitions. These transitions do not only act on the global topological parameters, but also on local descriptors, as well as on the crystallographical evolution.

Various types of topological transitions have been identified experimentally recently: pinch-off, ring collapse, ligament reattachment, and particle detachment and reattachment. The relative weight of such transitions to happen, seems to depend strongly on the material's solid volume fraction, but also on the coarsening stage.

We report on in-situ xray nanotomography experiments, that allowed for tracking same sample subvolumes, in order to further elucidate aspects of the topological evolution in bicontinuous metallic materials.

MM 8.4 Mon 12:30 C 230

Reversible mechanical actuation of nanoporous gold modified by electroactive self-assembled monolayers: Impact of the surface stress — •Olga Matts[1], Xinyan Wu[2], and Nadiia Mameka[1] — [1]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Hamburg University of Technology, Hamburg, Germany

Hierarchical nanoporous (hc np) metals made by dealloying present novel opportunities for the development of light-weight, high surface-area materials with diverse functionalities in the fields of catalysis, energy storage, sensing, and actuation. Most hc np metals possess a bimodal pore size distribution, featuring pores of hundreds of nanometers with nanometer-sized pores located within their walls. Understanding the impact of the porous hierarchy on functional behavior of hc np materials is crucial to further enhance their performance. This work reports the actuation in np-Au with single and bimodal size distributions modified by ferrocene-terminated alkanethiol self-assembled molecules (SAMs). For this, in situ dilatometry and cantilever bending are employed in electrolyte under potential control, exploiting the ability of the electroactive molecules to undergo reversible redox reactions. Pronounced variations in the macroscopic length change of the hybrids are revealed in response to the voltage-induced redox transformations. The phenomenon can be explained by a reorientational motion of the alkyl chains and the ferrocene-moiety due to uptake of electrolyte's anions. The steric hindrance and local disorder in the SAM clamped to the gold surface induces the surface stress, that is compensated by the bulk stress, and results in the actuation of the hybrid.

MM 8.5 Mon 12:45 C 230

Mitigation strategies for self-detachment of nanoporous thin films — •Gideon Henkelmann[1], Xinyan Wu[1,2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Optical and Electronic Materials, Hamburg University of Technology, Germany — [3]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum 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. Finally, we provide strategies to mitigate the self-detachment effect supported by both simulation and experimental results.

MM 9: Invited Talk: Markus Stricker

Time: Monday 15:00–15:30 Location: C 130

Invited Talk MM 9.1 Mon 15:00 C 130

Materials Informatics - appreciation of data and algorithms — •Markus Stricker — Ruhr-Universität Bochum

The foundation of the scientific method is reliable data. Digitalization in all parts of our society provides more and more accessible data. The amount and quality of available data, however, need new approaches to use the contained knowledge to its full potential. Within Materials Science these new methods are developed and applied in the sub-field of Materials Informatics. I will provide an overview of the current state of Materials Informatics and discuss applications of how data and algorithms are used to improve the description, characterization, discovery, and optimization of materials. Concrete examples include data fusion from experiments and simulations, active learning for materials discovery, and how latent knowledge in scientific texts can be efficiently used by employing natural language processing.

MM 10: Topical Session: Hydrogen in Materials: from Storage to Embrittlement I

Time: Monday 15:45–18:00 Location: C 130

Topical Talk MM 10.1 Mon 15:45 C 130

Unraveling the impact of defect-induced phases on hydrogen embrittlement and storage — •Ali Tehranchi[1], Poulami Chakraborty[1,2], Marti Lopez Freixes[1], Jing Rao[1], Maria J Duarte Correa[1], Baptiste Gault[1,3], Tilmann Hickel[1,4], and Jörg Neugebauer[1] — [1]-Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Basque Center for Applied Mathematics, Bilbao, 48009, Spain — [3]-Department of Materials, Imperial College, South Kensington,London, SW7 2AZ, UK — [4]Bundesanstalt für Materialforschung und -prüfung (BAM)

Establishing a hydrogen economy to reduce carbon emissions has sparked renewed interest in hydrogen embrittlement (HE) and hydrogen storage (HS) mechanisms. We examine the critical role of defect-induced hydride and metallic phases, highlighting associated challenges and opportunities. First, using ab initio thermodynamics the role of H on the relative stability of the fcc/bcc/hcp phases in steels is studied. These studies show the existence of a few atomic percent of H in retained austenite (RA) at experimentally relevant H chemical potentials. Therefore, a phase transformation of H-charged fcc to bcc will release the excess H. We discuss the interplay of H in grain/phase boundaries to assess the role of these excess H in HE. Second, the formation of nano-hydrides (NHs) in vicinity of various defects in ferritic FeCr and high-strength Al-based alloys is analyzed. NHs under indentors and around dislocations significantly alter the mechanical response of FeCr alloy. NHs in the vicinity of dislocations and micro-cracks in Al-based alloys provide new opportunities for enhancing HS.

MM 10.2 Mon 16:15 C 130

Strengths and Weaknesses of Classical Interatomic potentials for Hydrogen Embrittlement — •Ram Mohan Tirunelveli Vallinayagm[1,2], Elena Akhmatskaya[1,3], Iban Quintana[2], and Mauricio Rincon Bonilla[1] — [1]BCAM-Basque Center for Applied Mathematics, Alameda de Mazarredo 14, E-48009 Bilbao, Spain — [2]IK4-Tekniker, Surface Engineering and Materials Science Unit, Eibar, Spain — [3]IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, 48009 Bilbao, Spain

Molecular Dynamics is a common computational approach to probe the Hydrogen Embrittlement (HE) of steels at the atomistic scale. The reliability of these simulations depends on the interatomic potentials (IPs) describing particle interactions. A large number of IPs have been developed for the H-Fe system, yet no systematic benchmarking has been reported to date. Here, seven widely used IPs were benchmarked on the basis of four metrics, each critical to predicting HE: H-distribution, H-Diffusivity, Mechanical properties and H/grain boundary interactions. We put forward a classification scheme that allows practitioners to quickly choose the best IP for a particular application. The EAM potential by Song et al (Nat. Mater, 12, 145) was found to be the most adequate across the board, leading to reasonable predictions in each metric. Interestingly, we observed that other EAM IPs produce unrealistic H agglomeration, leading to long equilibration times and consistent underestimation of the H diffusivity. Poor performance of examined Modified EAM and Bond Order IPs could be due to the lack of H transport data during training.

MM 10.3 Mon 16:30 C 130

Effect of mechanical stress, chemical potential, and coverage on hydrogen solubility during decohesion of ferritic steel grain boundaries — Abril Azocar Guzman[1] and •Rebecca Janisch[2] — [1]IAS-9, Forschungszentrum Jülich, 52425 Jülich, DE — [2]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, DE

Hydrogen embrittlement (HE) mechanisms in structural materials such as iron and iron alloys present a complex scenario, in which the interaction of H with different crystal defects and the solubility of H in the system depends on the concentration, chemical potential and applied mechanical stress. Therefore, understanding these processes at the atomic level is fundamental for developing methods that can mitigate the detrimental effects of H. Grain boundaries (GBs) play a critical role in hydrogen enhanced decohesion mechanism, where H weakens the interatomic bonds causing intergranular fracture. In this work, we carry out DFT calculations to investigate the decohesion of the $\Sigma5(310)[001]$ and $\Sigma3(112)[1\bar{1}0]$ symmetrical tilt GBs in bcc Fe. To address the aforementioned open questions regarding the solubility of H, both thermodynamic limits of the separation of segregated interfaces are analysed. The results indicate that at higher local concentrations, H leads to a significant reduction of the cohesive strength of the GB planes, more pronounced at the $\Sigma5$ GB due to a more open local atomic environment. However, at higher applied mechanical stress and chemical potential, the solubility becomes higher at the $\Sigma3$ GB. To proceed from Fe to ferritic steel, also the effects of the alloying elements C, V, Cr and Mn at the GB are studied.

MM 10.4 Mon 16:45 C 130

The effect of solute atoms on the bulk and grain boundary cohesion in Fe: Implications for hydrogen embrittlement — •Poulami Chakraborty, Mauricio Rincon Bonilla, and Elena Akhmatskaya — Basque Centre for Applied Mathematics, Bilbao, Spain

Hydrogen embrittlement includes the mechanisms by which hydrogen diffuses in a system and causes mechanical degradation by loss of ductility. Therefore, in structural metals including Fe, selective alloying is used for strengthening and reducing the diffusivity of hydrogen by formation of precipitates or intermetallic phases which act as potential trapping sites. We have performed ab initio calculations focusing on the interactions of several alloying elements Cr, Ni, Mn commonly used in austenitic steels with grain boundaries. Our calculations helped us to identify alloying elements with the highest stabilising power. This is quantified by the calculation of thermodynamic parameters such as segregation and embrittlement energy. We have then compared these parameters in presence of hydrogen. Our systematic investigation enables us to understand the basic mechanism of hydrogen interaction with defects in alloys. Identification of such trends in presence of hydrogen can guide experimentalists in the choice of alloying elements and ultimately advance materials design.

MM 10.5 Mon 17:00 C 130

Hydrogen-driven surface segregation in Pd-alloys from atomic scale simulations — •Pernilla Ekborg-Tanner and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Pd-based nanoalloys show great promise as plasmonic hydrogen sensors. Nanoalloys are, however, subject to issues related to the chemical order such as surface segregation. The surface composition is directly related to the kinetic properties necessary for H sensing and as such, understanding the surface segregation during fabrication, operation and storage is crucial to ensure long-term stable sensors. In this work, we employ cluster expansions of PdAu and PdCu surface alloys with variable H coverage, trained using DFT calculations and sampled in Monte-Carlo simulations. This approach allows us to study the H coverage and the layer-by-layer composition of the near-surface region as a function of bulk composition, temperature and H pressure. We find that in the case of AuPd, Au segregates to the surface in vacuum while Pd segregates to the surface at full H coverage, and the transition between these regimes occurs over a narrow H pressure interval. In the case of CuPd, on the other hand, the H coverage varies much more gradually with H pressure and and is coupled to a non-monotonic variation of the Cu concentration in the topmost surface layer. The results demonstrate the rich behavior that can result from the coupling of metal-metal and metal-hydrogen interactions at surfaces, even in apparently simple but concentrated systems.

MM 10.6 Mon 17:15 C 130

Unveiling Synergies between Theory and Experiment for an Enhanced Understanding of Solid-State Hydrogen Storage — •Paul Jerabek[1], Thomas Klassen[1,2], and Claudio Pistidda[1] — [1]Abteilung für Materialdesign, Institut für Wasserstofftechnologie, Helmholtz-Zentrum Hereon, 21502 Geesthacht — [2]Helmut-Schmidt-Universität, Holstenhofweg 85, 22043 Hamburg

Metal hydride materials are a cornerstone for the secure and efficient storage of hydrogen in a versatile manner and play a pivotal role in realizing a carbon-emission-free transition energy. This underscores the need for a profound understanding of their material properties like stability against outside influences, (de)hydrogenation thermodynamics and kinetics across various length scales.

This contribution provides an overview of our journey to comprehend the fundamental principles of hydrogen storage within metal hydride materials, employing a combination of experimental and theoretical methods. The focus is on the intricate challenges inherent in this approach.

The collaborative synergy between theoretical frameworks, spanning from the atomistic to the mesoscopic scale, and experimental endeavors at our research center is highlighted. Concrete examples illustrate how DFT contributes to exploring interface properties of different hydrides and enable predictions of material stability against cosmic radiation. Additionally, this talk offers insights into how machine-learning techniques can drive progress toward a better understanding of solid-state hydrogen storage in various application scenarios.

MM 10.7 Mon 17:30 C 130

LaNi5 intermetallic compound for hydrogen storage in space applications; Theoretical investigation of material stability and dynamics — •Archa Santhosh[1], Thomas Klassen[1,2], Paul Jerabek[1], and Claudio Pistidda[1] — [1]Helmholtz-Zentrum Hereon GmbH, Max-Planck Strasse 1, 21502 Geesthacht — [2]Helmut-Schmidt-Universität, Holstenhofweg 85, 22043 Hamburg

LaNi5 intermetallic compound is a well studied hydrogen storage material owing to the good kinetics, high volumetric storage capacity and safety aspects. However, application in a space environment presents unique challenges concerning radiation exposure and subsequent material stability that needs to be understood further. In this work, we employed a combination of density functional theory (DFT) and molecular dynamics (MD) calculations to study the long-term stability of LaNi5 and its hydride phases when exposed to low-energy ionizing radiation. Valuable insights on primary damage events were obtained with MD calculations and the mechanism of defect formations, energetics, and the impact of defects on the electronic structure and stability were studied. The complexity and computational cost of the calculations were reduced by training a machine-learned (ML) interatomic potential and thereby coupling large-scale MD with ab-initio methods. This work further contributes a fundamental understanding of radiation tolerance and the subsequent suitability of LaNi5 alloys for hydrogen storage under the harsh conditions in space.

MM 10.8 Mon 17:45 C 130

Multiscale Modeling Metal-Hydride Interphases: Deconvoluted Chemo-Mechanical Energy for Phase-Field Simulations. — •Ebert Alvares[1], Kai Sellschopp[1], Bo Wang[2], Shinyoung Kang[2], Thomas Klassen[3], Tae Wook Heo[2], Paul Jerabek[1], and Claudio Pistidda[1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, Max-Planck-Straße 1, D-21502 Geesthacht, Germany — [2]Materials Science Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA — [3]Helmut Schmidt University, Holstenhofweg 85, 22043 Hamburg, Germany

Understanding the multiscale factors of the interphase boundary properties between metal-hydrides is crucial for simulating the hydrogenation process. It influences the hydride's stability, its rate of precipitation, and its morphology, thereby affecting the kinetics of transformation.

In this study, based on first-principles, thermodynamic models and micromechanical analysis were employed to deconvolute the interconnected chemo-mechanical components of the interphase boundary energy in the FeTi-H system, showing its application within an under-development quantitative-based phase-field model.

This generalizable approach offers valuable insights into the interplay between chemical and elastic contributions to any interstitial hydride formation, holding significant implications for the integration of micromechanics into phase field simulations of FeTi alloy hydrogenation, an ongoing research focus in our group.

MM 11: Data Driven Material Science: Big Data and Workflows II

Time: Monday 15:45–18:00 Location: C 243

MM 11.1 Mon 15:45 C 243

Leveraging Multi-Fidelity Data In AI-Driven Sequential Learning of Materials Properties: Identifying Stable Water-Splitting Catalysts — •Akhil S. Nair, Lucas Foppa, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin, Germany

The sequential learning of materials properties can enable a cost-effective materials discovery by iteratively extending the training data guided by an AI model [1]. Such an approach balances the exploitation of the model and the exploration of unvisited regions of the materials space. However, the efficiency of sequential learning relies on the performance of the AI model and on the quality of the data used to train the models. In material science, high-quality data is typically scarce. To address this challenge, we develop a sequential learning framework which utilizes low-fidelity data to improve the performance of the AI models for high-fidelity materials properties. In particular, we employ the symbolic regression based sure-independence screening and sparsifying operator (SISSO) method, which is suitable for small data sets and can better capture the behaviour of unseen materials compared to widely used AI methods [2]. Our approach is demonstrated for the discovery of stable oxide catalysts for water splitting, a process of significant importance in sustainable hydrogen production. For this, low and high-fidelity data are obtained from DFT-PBE and DFT-HSE calculations, respectively.

MM 11.2 Mon 16:00 C 243

From ab-initio to scattering experiments using neuroevolution potentials — •Eric Lindgren[1], Adam Jackson[2], Zheyong Fan[3], Christian Müller[4], Jan Swenson[1], Thomas Holm-Rod[5], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, United Kingdom — [3]College of Physical Science and Technology, Bohai University, Jinzhou, People's Republic of China — [4]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden — [5]ESS Data Management and Software Center, Copenhagen, Denmark

Machine-learned interaction potentials have in recent years emerged as an appealing alternative to traditional methods for obtaining forces for molecular dynamics simulations, combining the computational efficiency of semi-empiricial potentials with the accuracy of ab-inito methods. In particular, Neuroevolution potential (NEP) models, as implemented in the GPUMD package, are highly accurate and computationally efficient, enabling large scale MD simulations with system sizes up to millions of atoms with ab-initio level accuracy. In this work, we present a workflow for constructing and sampling NEPs using the 'calorine' package, and how the resulting trajectories can be analysed with the 'dynasor' package to predict observables from scattering experiments. We focus on our recent work on crystalline benzene as an example system, but the approach is readily extendable to other systems.

MM 11.3 Mon 16:15 C 243

Multi-Objective Optimization of Subgroups for the Discovery of Exceptional Materials — •Lucas Foppa and Matthias Scheffler — The NOMAD Laboratory at the FHI of the MPG and IRIS-Adlershof of the HU Berlin, Germany

Artificial intelligence (AI) can accelerate the design of materials by identifying correlations and complex patterns in data. However, AI methods commonly attempt to describe the entire, practically infinite materials space with a single model, whereas different mechanisms typically govern the materials behaviors in different regions of materials space. The subgroup-discovery (SGD) approach identifies local rules describing exceptional subsets of data with respect to a given target of interest. Thus, SGD can focus on mechanisms leading to exceptional performance.[1] However, the identification of appropriate SG rules requires a careful consideration of the generality-exceptionality tradeoff. Here, we analyse the tradeoff between exceptionality and generality of rules based on a Pareto front of SGD solutions.[2]

[1] B.R. Goldsmith, *et al.*, *New. J. Phys.* **19**, 013031 (2017).
[2] L. Foppa and M. Scheffler, arXiv.2311.10381 (2023).

MM 11.4 Mon 16:30 C 243

From Prediction to Action: Critical Role of Performance Estimation for Machine-Learning-Driven Materials Discovery — •Lucas Foppa[1], Mario Boley[2], Felix Luong[2], Simon Teshuva[2], Daniel Schmidt[2], and Matthias Scheffler[2] — [1]The NOMAD Laboratory at the FHI of the MPG and IRIS-Adlershof of the HU Berlin, Germany — [2]Department of Data Science and AI, Monash University, Australia

The development of machine-learning models for materials properties focuses on improving the average predictive performance of the models with respect to some training-data distribution. However, a good performance in average might not translate into an efficient discovery of materials via model-driven blackbox optimization (e.g., Bayesian). In these iterative materials-discovery approaches, the training data is extended based on a model-informed acquisition function whose goal is to maximize a cumulative *reward* over iterations, such as the maximum property value discovered so far. Crucially, the rewards might be decoupled from the average predictive performance, as they can be dictated by the model performance for the few exceptional materials of interest. Here, we illustrate this problem for the example of bulk-modulus maximization in perovskites and propose an estimator that recovers qualitative aspects of the actual rewards and can be computed using the intial training data.[1]

[1] M. Boley, *et al.*, arXiv:2311.15549 (2023).

15 min. break

MM 11.5 Mon 17:00 C 243

A generic Bayesian Optimization framework for the inverse design of materials — •Zhiyuan Li, Yixuan Zhang, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt Germany

The traditional approach to develop materials relies on the time- and resource-costly trial-and-error experiments, as well as phenomenological theory with limited predictivity. Despite recent advances in high-throughput density functional theory calculations and statistical machine learning techniques, it is still a big challenge to efficiently explore a vast chemical space with a small number of initial samples to identify materials with optimized properties.

In this study, we propose and implement a comprehensive inverse design framework based on Bayesian optimization, integrating feature engineering, surrogate models, and acquisition functions, aiming to expedite the process of materials discovery. Focusing on the intrinsic physical properties such as formation energy, hardness, band gaps, and magnetization, it is demonstrated how such a framework can be applied to recommend optimal compositions in a vast chemical space exhibiting desired properties.

MM 11.6 Mon 17:15 C 243

Uncertainty quantification by shallow ensemble propagation — •Matthias Kellner and Michele Ceriotti — École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Statistical learning algorithms provide a generally-applicable framework to sidestep time-consuming experiments, or accurate physics-based modeling, but they introduce a further source of error on top of the intrinsic limitations of the experimental or theoretical setup. One way to estimate this error is uncertainty estimation which make application of data-centric approaches more trustworthy. To ensure that uncertainty quantification is used widely, one should aim for algorithms that are reasonably accurate, but also easy to implement and apply. In particular, including uncertainty quantification on top of an existing model should be straightforward, and add minimal computational overhead. Furthermore, it should be easy to process the outputs of one or more machine-learning models, propagating uncertainty over further computational steps. We compare several well-established uncertainty quantification frameworks against these requirements, and propose a practical approach, which we dub shallow ensemble propagation, that provides a good compromise between ease of use and accuracy. We present applications to the field of atomistic machine learning for chemistry and materials, which provides striking examples of the importance of using a formulation that allows to propagate errors without making strong assumptions on the correlations between different predictions of the model.

MM 11.7 Mon 17:30 C 243

Extracting physics with feature selection: How much data do we need and what can we really learn? — Guido Gaggl, Johannes C. Cartus, and •Oliver T. Hofmann — Institute of Solid State Physics, TU Graz

Feature selection algorithms such as SISSO allow a quick and automated analysis of data with the aim to find an equation that relates a target property of a system with properties of its constituent. Ideally, this equation coincides with the correct underlying physics. Unfortunately, this is often not the case, but even then, analyzing which constituent properties appear is often used to identify promising features. In this work, we analyze how well SISSO performs this task adverse circumstances. First, we demonstrate that given enough high-quality data and a sufficiently large feature space, it is indeed able to recover the correct physical equation. This is also surprisingly robust when reducing the number of available data points, even when including random or systematic bias into it. Conversely, adding even relatively small amount of noise to the data quickly deteriorates the performance. Finally, we discuss that in situations where two physical effects are superimposed, SISSO is intrinsically unable to find either, even when including multiple rungs.

MM 11.8 Mon 17:45 C 243

Adaptive-precision potentials for large-scale atomistic simulations — •David Immel[1,2], Ralf Drautz[1], and Godehard Sutmann[1,2] — [1]ICAMS, Ruhr-Universität Bochum, Bochum, Germany — [2]JSC, Forschungszentrum Jülich, Jülich, Germany

Large-scale atomistic simulations rely on interatomic potentials providing an efficient representation of atomic energies and forces. Modern machine learning (ML) potentials provide the most precise representation compared to electronic structure calculations while traditional potentials provide a less precise, but computationally much faster representation and thus allow simulations of larger systems.

We combine a traditional and a ML potential to a multi-resolution description, leading to an adaptive-precision potential with an optimum of performance and precision in large complex atomistic systems. The required precision is determined per atom by a local structure analysis and updated automatically during a simulation. We use Copper as demonstrator material with an embedded atom model (EAM) as traditional and an atomic cluster expansion (ACE) as ML potential, but any material and potential combination can be used for an adaptive-precision potential. The approach is developed for the molecular dynamics simulator LAMMPS and includes a load-balancer to prevent problems due to the atom dependent force-calculation times, which makes it suitable for large-scale atomistic simulations.

In this contribution strategies for the creation of an adaptive-precision potential are discussed. First results from Copper nanoindentations are reported and further improvements are outlined.

MM 12: Materials for Storage and Conversion of Energy III

Time: Monday 15:45–16:45 Location: C 264

MM 12.1 Mon 15:45 C 264

The EFG Rosetta Stone: Translating between DFT simulations and Solid State NMR experiments — •Javier Valenzuela Reina[1], Simone Köcher[2,1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy and Climate Research (IEK-9), Forschungszentrum Jülich

Solid-state Nuclear Magnetic Resonance (NMR) spectroscopy is an accurate, non-destructive method for the analysis of solid-state materials. However, the spectra of complex compounds, like battery materials, are usually challenging to interpret, due to disorder or amorphous phases. Predictive-quality simulations of NMR observables are therefore crucial for an unambiguous interpretation. Unfortunately, calculating NMR properties of solid-state materials is a non-trivial task. This holds particularly for the battery-relevant quadrupolar ^{7}Li isotope, which experiences additional interactions between the nuclei and the surrounding electric field gradient (EFG).

In this work, we evaluate the performance of plane-wave density-functional theory (DFT) to compute the quadrupolar coupling constants (C_Q) and asymmetry parameters (η) of different lithium salts. The impact of unit cell size, geometry, and details of the simulation strategy is assessed, and the accuracy of the results is compared to NMR of other nuclei such as aluminium.

The reference scale we thereby introduce is a valuable resource for interpreting and validating further NMR experiments and simulations.

MM 12.2 Mon 16:00 C 264

Application and pitfalls of self-measured EELS standards on a Cu based MeOH catalyst for oxidation state determination — •Daniela Ramermann, Lukas Pielsticker, Michael Poschmann, Christoph Göbel, Elisabeth H. Wolf, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim (Ruhr)

Electron energy loss spectroscopy (EELS) is a powerful technique, not only for the determination of the elemental composition, but also for the investigation of chemical bonding and oxidation states. For the analysis of EELS data, the use of cross-section models is quite common. However, the use of reference spectra (standards) improves the quantification results and in addition allows for the fitting of the edge shapes to investigate phase composition / oxidation states. Such standards are obtained from acquired materials of well-known and defined properties. There are several databases for EELS references [1], however, their content is not exhaustive.

To apply this principle on our samples, we obtained a set of well-defined materials for the acquisition of EELS reference data. As these materials may have local impurities and differ from the desired oxidation state, it is crucial to ensure that these materials are in a well-defined state. We show the process of acquiring suitable EELS standards for materials used in catalysis and the application of mapping the oxidation state and phase composition on a Cu based methanol synthesis catalyst.

[1] https://eelsdb.eu, https://eels.info/atlas, http://eel.geri.re.kr

MM 12.3 Mon 16:15 C 264

Piezoresponse force microscopy on $BaTiO_3$ based relaxors — •Markus Kratzer[1], Philipp Münzer[1], Christian Maier[3], Klaus Reichmann[3], Marco Deluca[2], and Christian Teichert[1] — [1]Chair of Physics, Montanuniversität Leoben, Leoben, AUT — [2]Materials Center Leoben, Leoben, AUT — [3]Institute for Chemistry and Technology of Materials, TU Graz, Graz, AUTGraz,

Electrical energy storage systems with high energy- and power density are of great interest in electronics. A possible material choice to realize such devices are relaxor ceramics. Lead-free examples are $BaTiO_3$ based systems, where the relaxor behavior is obtained via the disruption of the ferroelectric long-range order by replacing Ti^{4+} by homo- or heterovalent substitutes in $BaTiO_3$'s perovsike unit cell. Here, the microscopic ferroelectric behavior of $BaTiO_3$ with increasing amounts of Zr^{4+} and Nb^{5+} has been investigated utilizing piezo response force microscopy. The investigations reveal that the disruption of the ferroelectric long-range order is highly sensitive to the amount and type of substitutes.

MM 12.4 Mon 16:30 C 264

Chlorine-induced high-temperature corrosion of superheater steels — •Matthias Kroh, Georg Krupkov, Sebastian Pentz, and Ferdinand Haider — Univ. Augsburg, Inst. f. Physik, 86159 Augsburg

The combustion process in waste-incineration-plants releases a variety of chemical substances into the gas stream. Under the operational environment Cl2 and HCl cause the Chlorine-catalysed high-temperature corrosion, which is a driving factor in the degradation of the overheater tubes necessary for power generation. Literature suggests that molecular Chlorine is the far more aggressive species, although the conducted studies were of a more qualitative nature and did not take the real conditions in power plants into consideration. To further distinguish the effect of the two species either HCl or Cl2 was let flow directly into the setup. Thereby the Cl2 was produced using a Chlorine generator, in which the reaction of liquid NaOCl and H2SO4 releases Cl2 in the process. The Chlorine concentrations were quantified by GCMS and UV VIS spectrometry, whilst the concentration of HCl was quantified through ISE measurements. In these experiments the corrosive attack of Cl2 and that of HCl on samples of a typical superheater steel was determined for various temperatures and defined gas atmospheres. The experimental setup consists of a horizontal furnace, where the samples were exposed to a flow of the desired gas atmosphere, followed up by a 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 13: Phase Transformations I

Time: Monday 15:45–16:45 Location: C 230

MM 13.1 Mon 15:45 C 230

Impact of magneto-chemical coupling on phase stability, vacancy formation and atomic diffusion in Fe-Cr alloys — •Hilal Bozkurt[1], Chu-Chun Fu[1], and Cyrille Barreteau[2] — [1]CEA, SRMP, Gif-sur-Yvette, France — [2]CEA, CNRS, SPEC, Gif-sur-Yvette, France

High chromium ferritic steels present a large variety of technological applications. For instance, they are promising candidate as structural materials for future fusion reactors, thanks to their strong resistance to corrosion and to radiation damage. On the other side, it is known from numerous studies that thermodynamic and kinetic properties of Fe-Cr alloys are highly sensitive to magnetism.

Despite the large amount of previous theoretical and experimental efforts, the impact of magnetism on vacancy formation and vacancy-mediated diffusion in Fe-Cr as a function of temperature and alloy composition is still unclear.

In this work, we first investigate the dependency of vacancy formation energy and migration barriers on the magnetic and chemical configuration of Fe-Cr alloys, via first principles calculations. The obtained data are then used to parameterize a spin-atomic Monte Carlo model, in order to perform simulations for an accurate prediction of equilibrium vacancy concentration and vacancy-mediated atomic-diffusion coefficients versus temperature. The specificity of the present model consists in an explicit treatment of both chemical and magnetic variables, which enables to elucidate the impact of the magneto-chemical interplay on the studied properties.

MM 13.2 Mon 16:00 C 230

Ab initio study of structure-property relations in Pb-supersaturated Sn-rich Pb-Sn alloys — •Martin Friák[1], Petr Čípek[2,1], Jana Pavlů[2], Ondřej Zobač[1], Pavla Roupcová[1,3], Ivana Miháliková[1], David Holec[4], Šárka Msallamová[5], and Alena Michalcová[5] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Rep. — [2]Masaryk University, Brno, Czech Rep. — [3]CEITEC Brno University of Technology, Brno, Czech Rep. — [4]Montanuniversität Leoben, Leoben, Austria — [5]University of Chemistry and Technology in Prague, Prague, Czech Rep.

We have performed a theoretical study of three different allotropes of Pb-supersaturated Sn-rich Pb-Sn alloys with the α-Sn, β-Sn and a simple hexagonal γ-Sn structure employing quantum-mechanical calculations. Structure-property relations were analyzed in the case of the lattice parameters, thermodynamic stability, elastic properties and mechanical stability as well as electronic-structure density of states. Compositional trends in structural, thermodynamic and electronic-structure properties were found nearly linear. Our theoretical study sheds new light on a decades-long controversy related to the γ-phase of supersaturated Sn-rich Pb-Sn alloys reported in earlier papers. We suggest that the experimental difficulties in synthesizing the γ-phase solid solutions are due to the high formation energy of this phase. A financial support received under the Project No. 22-05801S from the Czech Science Foundation is gratefully acknowledged.

MM 13.3 Mon 16:15 C 230

The impact of spin-polarization, atomic ordering and charge transfer on the stability of CoCrNi alloy — •Pavel Papež[1,2], Martin Zelený[1], Martin Friák[2], and Ivo Dlouhý[1,2] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, Žižkova 22, Brno, 616 00, Czech Republic

Our theoretical study analyzes the impact of atomic ordering, magnetization and ongoing charge transfer on the phase stability of the medium entropy CoCrNi alloy. The study was performed using ab-initio calculations employing simulation supercells containing 216 atoms. The supercells contained either fcc or hcp lattice sites as obtained by changing the stacking of atomic planes. For each lattice type we used six different distributions of atoms with different levels of ordering. For charge transfer analysis we employed the method developed by R. Bader. To evaluate the phase stability we have calculated the mixing enthalpy of the structures revealing differences caused by ordering. Regarding the impact of the 1st nearest neighbours (NN) on the local magnetic moments of atoms, we found clear trends in Co, Cr and Ni atoms depending on the 1st NN Cr atoms. The charge transfer exhibits similarly clear trends in which Cr releases its electrons to the two other elements and even this effect has clear dependence on Cr in 1st NN (for details see P.Papež et al., Mater. Chem. Phys. 304 (2023) 127783, https://doi.org/10.1016/j.matchemphys.2023.127783)

MM 13.4 Mon 16:30 C 230

Phase diagram of the incommensurate magnetic Hubbard model — •Liam Rampon[1], Fedor Šimkovic IV[3], and Michel Ferrero[1,2] — [1]CPHT, CNRS, École Polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — [2]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France — [3]IQM, Nymphenburgerstr. 86, 80636 Munich, Germany

We present the magnetic phase diagram of the cubic Hubbard model at strong coupling. We investigate the onset of spin-spiral orderings as a function of temperature and for dopings up to 20%. By computing relevant thermodynamical potentials, we identify the leading ordering vector and discuss the mechanism that gives rise to the ordered state. We observe manifestations of the Pomeranchuk effect and also show strong evidence for a phase separation at lower temperature and doping, possibly caused by an underlying "stripe" phase. These findings were obtained with single-site dynamical mean-field theory, using a broken-symmetry formalism that allows one to directly stabilize incommesurate spiral orders.

MM 14: Materials for Storage and Conversion of Energy IV

Time: Monday 16:45–18:00 Location: C 264

MM 14.1 Mon 16:45 C 264

Pressure Induced Oscillating Band-gap Variation in KBaTeSbO6 : Towards Transparent Solar Cell — •Manasa Gattavadi Basavarajappa[1], Diwakar Singh[2], and Sudip Chakraborty[1] — [1]Harish-Chandra Research Institute,Chhatnag Road, Jhunsi, Prayagraj, India 211019 — [2]University of Duisburg-Essen, Essen, North Rhine-Westphalia, Germany

Recently, double oxide perovskites have emerged as a group of promising materials for wide range of applications due to their unique electronic and optical properties. There has been substantial studies establishing the fact that employment of external stimuli such as pressure on these materials may lead to drastic change in their properties, further enhancing their usefulness.

In this work, we have studied various pressure-induced structural, electronic and optical properties in an extended double oxide perovskite, KBaTeSbO6. Our study reveals the occurrence of band-gap tuning via blue shift followed by a red shift in KBaTeSbO6 with external pressure. This transition leads to modified electronic properties. We observed distinct structural changes under pressure such as lattice compression, distortion and phase transition. Our results indicates that the pressure-induced changes in band structure and lattice parameters directly affects the optical properties, resulting in altered absorption and reflection spectra. In order to validate the realisation of the material, we have also studied the formation and thermodynamic stability of the material under various pressure.

MM 14.2 Mon 17:00 C 264

Unveiling the Electronic and Structural Properties of Phosphonium- Based Perovskites: A First Principle Study Using Density Functional Theory — •Arijeet Sarangi and Sudip Chakraborty — Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj, India 211019

Phosphonium-based perovskites have emerged as promising materials for various electronic and optoelectronic applications due to their unique electronic and structural properties. In this study, we present a comprehensive investigation into the electronic and structural characteristics of phosphonium-based perovskites, aiming to shed light on their potential for enhancing device performance. Through DFT calculations, we explore the crystal structure, band gap engineering, charge transport, and optical properties of these materials. Our results provide valuable insights into the electronic band structure, density of states, and effective mass of charge carriers in phosphonium-based perovskites, enabling a deeper understanding of their optoelectronic behavior. Additionally, we explore the influence of defects and doping on the electronic properties and discuss their impact on device performance. Our findings provide valuable insights into the fundamental understanding of phosphonium-based perovskites, paving the way for their application in thin film solar cells, optoelectronic devices, and other emerging technologies. This study contributes to the ongoing research efforts towards harnessing the full potential of phosphonium-based perovskites and advancing the field of perovskite materials for sustainable energy solutions.

MM 14.3 Mon 17:15 C 264

Investigation of varied doping mechanism on the thermoelectric properties of pyrite FeS_2 — •Anustup Mukherjee and Alaska Subedi — CPHT, Ecole Polytechnique. Institut Polytechnique de Paris, Palaiseau, France - 91120

Pyrite FeS_2 is an earth-abundant, nontoxic sulphide mineral with semiconducting behaviour. Hence, it has been investigated for various energy applications, including thermoelectrics using experiments and theoretical studies. Large values of thermopower have been observed at room-temperature. However, there exists a discrepancy in the magnitude and sign of thermopower reported in the literature depending on the nature of sample. Co-doped FeS_2 samples show similar variations in the magnitude of room-temperature thermopower. Therefore, it is of immense importance to examine the intrinsic thermopower of self- and Co-doped FeS_2 systems. We have investigated the electronic structure, magnetism and thermoelectric transport properties of these systems using first-principles calculations. We have implemented three different doping schemes, namely explicit Co-substitution, jellium doping and electron addition within the rigid band approximation (RBA) picture to understand electron doping in FeS_2. The former two doping schemes take structural modification and charge screening into consideration which is absent in the simpler RBA method. The thermopower is overestimated within the RBA picture, however the room-temperature thermopower observed is under 50 μV/K for all the doping schemes, suggesting that electron doped FeS_2 is not a good candidate for thermoelectric applications.

MM 14.4 Mon 17:30 C 264

Ab-initio study of doping in silicon carbide — •Zahra Rajabzadeh and Lorenz Romaner — Department of Materials Science, Montanuniversität Leoben, Roseggerstraße 12, 8700 Leoben, Austria.

The wide band gap semiconductor SiC is an outstanding material for high-power electronics, e.g. for inverter applications in electric cars.. Although SiC is generally doped with elements such as N or Al, the fundamental properties of these point defects are still not understood.

We use density functional theory (DFT) calculations to investigate the impact of dopants on SiC properties focusing on the most relevant polytypes 3C, 6H, 4H and 2H. Calculations are carried out with the Vienna Ab- initio Simulation Package (VASP). We employ the PBE exchange-correlation functional with and without van der Waals (vdW) corrections as well as the HSE06 hybrid functional. First, we present results where a nitrogen or aluminum atoms are placed inside the crystal structure for different polytypes and the formation energy for different dopants are discussed. Then we will discuss binding energy for (N, Al) co-doping configurations. Furthermore, we explore concentration effects which allow studying the impact of non-stoichiometry on the formation energies. The results for all defects are analyzed also in terms of the electronic structure including band gaps and projected density of electronic states. Finally, we discuss nitrogen solubility to understand how much nitrogen can dissolved in SiC.

MM 14.5 Mon 17:45 C 264

A direct observation of the influence of nitrogen-doping on ion dynamics for electric double layer capacitor performance — •Henry R. N. B. Enninful[1,3], Marius Hermesdorf[2], Desirée Leistenschneider[2], Martin Oschatz[2], Alex Forse[3], and Rustem Valiullin[1] — [1]Universität Leipzig — [2]Friedrich-Schiller-Universität Jena — [3]University of Cambridge, UK

Substantial improvements in the design of Electric Double Layer Capacitors (EDLC) have led to increased performance in both power and energy densities. To obtain comparable energy densities to those of batteries, electrode materials functionalized with nitrogen have been produced to yield very high specific capacitances and energy densities.

The mechanisms that underlie the improved capacitances due to electrode-electrolyte surface interactions is still rarely understood. This work sheds light on ion transport and mobility at the pore surface and within the pore interior. We show that for carbon electrodes synthesized from cellulose and potassium carbonate, increased melamine content leads to a sacrifice of the pore surface area and volume, resulting in reduced specific capacitances. Furthermore, the substitution of melamine with urea in the same ratio produces reduced nitrogen content in the resulting material. The effect thereof, is an attendant reduction in specific capacitance regardless of the comparable surface area. Lastly, we show that electrodes with a certain threshold of nitrogen content are able to store ions from a pure water *electrolyte*. The phenomena resulting in the produced performances are explained and future prospects in this work are shown.

MM 15: Phase Transformations II

Time: Monday 16:45–18:00 Location: C 230

MM 15.1 Mon 16:45 C 230

Quantum hydrogen bond symmetrization in water ice and sulfur hydride — •Marco Cherubini and Michele Casula — Institut de Minéralogie, de Physique de Matériaux et de Cosmochimie, CNRS, Paris, France

Hydrogen bond symmetrization, influenced by the quantum nature of protons, is expected in various compounds. Nuclear quantum fluctuations diminish the boundary between symmetric and asymmetric phases by several gigapascals. Here, we investigate water ice and sulfur hydride, compounds exhibiting hydrogen bond symmetrization and sharing deep analogies. We use path integral molecular dynamics and the self-consistent harmonic approximation in combination with Quantum Monte Carlo, ab initio calculations, and machine learning potentials to solve the nuclear and electronic problems. In water ice, hydrogen bond symmetrization is a long-debated issue because of the lack of univocal experimental signatures. We describe, for the first time, the strong temperature dependence of the critical pressure in the classical regime, showing that quantum effects are so strong as to completely cover the thermal fluctuations, reducing the phase boundary by over 50 GPa. Importantly, we prove that proton disorder minimally influences quantum symmetrization. Sulfur hydride has been widely studied for its superconductivity, with its maximum critical temperature (200 K) previously believed to be associated with hydrogen bond symmetrization. Indeed, we prove that it is related to the transition from the symmetric phase to a phase characterized by disordered local moments, and that the asymmetric phase is reached at much lower pressures.

MM 15.2 Mon 17:00 C 230

Unusual spectral features in BaZrO3 — •Petter Rosander, Erik Fransson, Nicklas Österbacka, Paul Erhart, and Göran Wahnström — Chalmers university of technology, Gothenburg, Sweden

Barium zirconate $BaZrO_3$ is one of few perovskites that retains an average cubic structure down to 0 K at ambient pressure. Despite this, it shows unusually sharp features in the Raman spectrum, which are supposed to be absent in a cubic system. In addition, a sharp reflection in electron diffraction appears at the R-point of the crystal at low temperatures. It has been suggested that these features are due to that the local structure of $BaZrO_3$ may form nanodomains or a glass-like phase at low temperatures.

Here, the static structure factor of $BaZrO_3$ is calculated as a function of temperature and pressure via molecular dynamics simulations using a machine-learned potential with near density functional theory (DFT) accuracy. A dielectric tensor model is also trained with near DFT accuracy to calculate the Raman spectrum as a function of pressure using molecular dynamics simulations.

We show that the sharp features in the Raman spectrum is due to higher order scattering and that the sharp reflection observed in electron diffraction is diffuse superlattice reflections that stems from the onset of a phase transition that never occurs.

MM 15.3 Mon 17:15 C 230

Electronic and atomic structure analysis of $Fe_4(P_2O_7)_3$ crystal — •Svitlana Pastukh[1,2], Pawel Jochym[2], Dominik Legut[1], and Przemysław Piekarz[2] — [1]IT4Innovations, VSB-Technical University of Ostrava, 708 00 Ostrava, Czech Republic — [2]Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342 Kraków, Poland

This research delves into a comprehensive investigation of the electronic, magnetic, and structural characteristics of the $Fe_4(P_2O_7)_3$ crystal through first principles calculations utilizing DFT. Employing the GGA within VASP, our study focused on elucidating the properties of the crystal lattice, which adopts a monoclinic structure under space group $P2_1|n$. The optimized lattice parameters were determined as a=7.409 Å, b=21.425 Å, c=9.529 Å, with a unit cell containing four molecules (Z=4). It was shown that by taking into account van der Waals corrections, we aimed to improve the treatment of dispersion interactions and enhance the accuracy of the crystal structure optimization. Our examination encompasses the electronic and lattice attributes, considering four distinct magnetic configurations. The investigation revealed the AFM-1 configuration to possess the lowest total energy, exhibiting magnetic moments of 4.598 μ_B on Fe atoms. Additionally, for the relaxed crystal structure, we conducted analyses of the phonon dispersion relations and phonon density of states through the temperature-dependent effective potential method. These comprehensive findings contribute significantly to enhancing our understanding of the $Fe_4(P_2O_7)_3$ crystal, shedding light on its potential applications across various scientific domains.

MM 15.4 Mon 17:30 C 230

Phase transitions in 2D halide perovskites using machine learned potentials — •Erik Fransson, Julia Wiktor, and Paul Erhart — Chalmers University of Technology, Sweden

Two dimensional hybrid halide perovskite is a class of materials with interesting and useful optoelectronic properties for many applications areas, such as solar cells. These structure consists of one or a few layers of the perovskite phase connected via organic spacer molecules, and they can for example exhibit increased stability compared to their 3D counterparts.

Here, we make use of machine learning potentials, with near DFT accuracy, and large-scale molecular dynamics simulations in order to investigate thermodynamic properties and stability of these complex structures for the prototypical spacer molecule phenethylammonium (PEA). The phase transitions can directly be observed via structural parameters such as octahedral tilt angles and bond-lengths. Interestingly, we find that the phase transitions in the single perovskite layer structure appears at a significantly higher temperature and with different character compared to the 3D perovskite phase. We analyze the phase transitions temperature and character with varying number of perovskite layers in order to understand how the phase transition property changes as a function of dimensionality in the system. We observe surface effects for the thicker perovskite systems, such as the surface layers exhibiting stronger octahedral tilt and undergo the phase transitions at higher temperatures (about 50K) compared to the bulk-layers.

MM 15.5 Mon 17:45 C 230

MT6Z6 kagome candidates with flat bands, magnetism, phonon instability, and charge density waves — •Xiaolong Feng[1], Yi Jiang[2], Haoyu Hu[2], Dumitru Călugăru[3], Maia Garcia Vergniory[1,2], Claudia Felser[1], Santi Blanco-Canosa[2], and Bogdan Andrei Bernevig[2,3,4] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Donostia International Physics Center(DIPC), Paseo Manuel de Lardizábal. 20018, San Sebastián, Spain — [3]Department of Physics, Princeton University, Princeton, NJ 08544, USA — [4]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

Kagome materials manifest rich physical properties due to the emergence of abundant electronic phases at different fillings. Here, we carry out a high-throughput first-principles study of the MT6Z6 kagome materials, regarding their electronic flat bands and lattice instability. The diverse MT6Z6 kagome candidates reveal the remarkable tunability of kagome flat bands from unfilled and fully filled states. Mn/Fe-166 compounds exhibit partially filled flat bands with a pronounced sharp DOS peak near the Fermi level, suggesting the presence of magnetic orderings, which split the sharp DOS peak and stabilize the phonon. When the flat bands are located away from the Fermi level, the instabilities can be classified into three types, regarding their vibration modes. Type-I instabilities involve the in-plane distortion of kagome nets, while type-II and type-III present out-of-plane distortion of trigonal M and Z atoms. Our prediction suggests a vast kagome family for the exploration of rich properties induced by the flat bands.

MM 16: Poster Ia

Time: Monday 18:30–20:30 Location: Poster E

MM 16.1 Mon 18:30 Poster E

Investigation of excitation-induced non-thermal effects in semiconductors, metals and alloys — •Simon Kümmel and Johannes Roth — FMQ, Universität Stuttgart, Germany

Excitation-induced non-thermal melting in silicon, as well as bond-hardening in gold following strong laser irradiation with short pulse durations have been known for several years. Furthermore, several traces of excitation-induced solid-solid phase transitions have been noticed in a variety of materials.

Here, we present several approaches to identify and quantify excitationinduced effects changing the bond strength and inducing phase transitions systematically in several semiconductors, metals and alloys obtained from DFT calculations depending on the degree of excitation. These calculation are in line with previous investigations and provide new insights into the change of the bond strength and the induced phase transitions following strong laser excitation.

MM 16.2 Mon 18:30 Poster E

Ab initio study of transition paths between (meta)stable phases of Nb and Ta-substituted Nb — •Susanne Kunzmann[1,2,3], Thomas Hammerschmidt[3], Gabi Schierning[1,2,4], and Anna Grünebohm[3,5] — [1]Experimental Physics, Bielefeld University, Germany — [2]Research Center Future Energy Materials and Systems (RC FEMS), University of Duisburg-Essen, Germany — [3]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany — [4]Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany — [5]Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Despite being well-characterized, Niobium exhibits unexplained anomalies. To address this, we employ density functional theory to revisit the metastablephases of Nb and Nb with Ta impurities. We compare energies and groundstate volumes of selected crystal structures, explore potential transition paths to the bcc ground state and the energy landscape for tetragonal distortions. Additionally, we assess stability through phonon spectra and vibronic free energies. We discuss previously overlooked aspects: a new local energy minimum on the bcc to ω transition path, a flat energy landscape concerning uniaxial strainalong [111], and significant stabilization of the σ phase through Ta substitution.

MM 16.3 Mon 18:30 Poster E

Quantum Restored Symmetry Protected Topological Phases — •Dhruv Tiwari[1], Steffen Bollmann[1], Thomas Köhler[2], Sebastian Paeckel[3], and Elio J. König[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Uppsala University, Upsala, Sweden — [3]Ludwig Maximilian University, Munich, Germany

Symmetry Protected Topological phases are paradigmatic for the nontrivial interplay of topology, symmetry, and interactions. For a given group of symmetries, it is already known that the topological classification can be different for interacting and non-interacting systems. On the other hand, one usually resorts to a mean-field approximation to study interacting systems where the tools of non-interacting topology can be employed to study topological characteristics. This raises the natural question as to what is the role of quantum fluctuations in the topological characteristics of interacting systems. We present an example of a system that is trivial under the mean-field approximation and shows topological characteristics upon the introduction of quantum fluctuations. To this end, we present results on an array of topological Cooper pair boxes. At half-filling, we observe the restoration of topological characteristics upon the introduction of quantum fluctuations. At quarter-filling, we obtain a richer phase diagram once we take into account the contribution of quantum fluctuations.

MM 16.4 Mon 18:30 Poster E

Ab initio study of phase stability of YMn2 with different magnetic orderings — •Pavel Papež, Martin Friák, and Ilja Turek — Institute of Physics of Materials, Czech Academy of Sciences, Žižkova 22, Brno, 616 00, Czech Republic

Our work is focused on the intermetallic compound YMn2 which exhibits an anomalous thermal expansion. The origin of this phenomenon is belived to be magnetism-related but it is not completely understood yet. A puzzling aspect is e.g. a 5% volume change at the Neél temperature of 100 K. We have employed quantum-mechanical calculations to examine the thermodynamic stability of different magnetic states. Our calculations included non-collinear magnetic states which were defined employing the spin-orbit coupling. The computational cell was that of the C15 Laves phase and contained 24 atoms. The 7 different magnetic configurations were set up along the [0 0 1] direction. Our results show the most stable configuration is an antiferomagnetic (AFM) state which is followed closely by two experimentally reported configurations with the same AFM nearest neighbour configurations but pointing along different directions. Interestingly, these two magnetic configurations exhibit very similar energies. Importantly, the resulting magnetic moments on Mn atoms and lattice parameters show very good agreement with the values reported in previous experimental studies.

MM 16.5 Mon 18:30 Poster E

Investigating changes of chemical bonding upon charge density wave transition in CuTe — •Johannes Holters, Christian Stenz, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany

Properties of solids like the electrical conductivity, band gap, phonon dispersion and dielectric function are governed by the chemical bonds between the atoms. Changes in the bonding is thus indirectly measurable by electrical and optical means. The metallic mineral CuTe exhibits a Peierls-like distortion along tellurium chains below the transition temperature of 62°C. Due to the distortion the overlap of the Cu d-orbitals and Te p-orbitals is reduced, which leads to the occurence of a quasi-1D charge density wave. This work analyses the temperature-induced structural change of polycrystalline CuTe produced by sputter deposition by electrical and optical measurements. The electrical conductivity, phonon softening and dielectric function is used to investigate changes in the chemical bonding as a consequence of the electronic rearrangement along the Te-chains.

MM 16.6 Mon 18:30 Poster E

Phase transitions and electronic properties of Fe2O3 under laser compression by ultrafast in-situ X-ray absorption spectroscopy — Juan Pintor[1], Delphine Cabaret[2], and •Marion Harmand[3] — [1]IMPMC, Sorbonne University, Paris, France. — [2]IMPMC, Sorbonne University, Paris, France. — [3]IMPMC, Sorbonne University, Paris, France.

Understanding the structural changes in hematite (α-Fe2O3) under extreme pressure and temperature is essential for gaining insights into the physical properties of planetary interiors. At ambient conditions, hematite exhibits a rhombohedral structured antiferromagnetic insulator. Its high-pressure behavior has been extensively studied, with particular focus on pressures around 50 GPa, revealing a 10% volume cell drop, a change in crystal symmetry, a Mott transition, and the collapse of iron magnetic moments (high-spin to low-spin transition). The exact nature of the phase transition in this pressure range remains controversial, with debates about whether the electronic or structural transition drives the other. This study reports ultrafast time-resolved X-ray Absorption Near Edge Spectroscopy (XANES) measurements conducted at the High Power Laser Facility of ESRF-ID24 beamline. Our data capture time-resolved transformations, revealing changes in the different XANES features within hundreds of ps, after the shock breakout from the samples. This presentation will detail a time-resolved examination of XANES changes with respect to pressure and temperature. For further understanding of the XANES features, preliminary DFT calculations will also be presented.

MM 16.7 Mon 18:30 Poster E

Spin and phase state of iron in FeS at Martian core conditions — •G. Scholz[1], C. Albers[1], H. Gretarsson[2], G. Kovalskii[3], M. Mezouar[4], W. Morgenroth[3], L. Pennacchioni[3], J. Savelkouls[1], M. Sundermann[2], N. Thiering[1], M. Wilke[3], and C. Sternemann[1] — [1]TU Dortmund, Dortmund, Germany — [2]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [3]University of Potsdam, Potsdam, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

The Martian core is assumed to be comprised of molten FeNi with up to 15 wt% S and 5 wt% O. To further understand the electronic structure of iron, we investigated the changes in phase state and spin state in FeS, a simplified core composition, which are induced by high pressure (p) and high temperature (T).

In order to explore this topic, we conducted *in situ* (resonant) X-ray emission spectroscopy at beamline P01, PETRA III (DESY) using a von Hamos spectrometer. We used diamond anvil cells in combination with a double-sided Yb:YAG-laser heating setup to achieve pressure and temperature conditions up to 64 GPa and 3000 K, respectively. The phase state of FeS was evaluated at beamline ID27, ESRF with X-ray diffraction combined with double-sided *in situ* laser heating up to 43 GPa and 3000 K.

In both experiments, our focus was set on the temperature induced phase transition from FeS-III to -IV and -V and the potential spin state change at p/T-conditions of the FeS-IV and -V phase transition boundary.

MM 16.8 Mon 18:30 Poster E

Characterization and improvement of the hydrogen embrittlement properties of AM316L — •Kai Lagemann, Stefan Wagner, and Astrid Pundt — Karlsruher Institute for Technology (KIT), Institute for Applied Materials Materials Science and Engineering (IAM WK), Karlsruhe

In this project, powder bed-based laser melting (PBF-LBM) is used to investigate additively manufactured 316L steel, which is planned to be used as a structural material in hydrogen technology in the future. It is investigated how the microstructure changes through the application of a remelting (RM) strategy and whether printing defects can be minimised as a result.

The RM parameter study identifies optimal manufacturing parameters. It is shown that the RM strategy melts remanent powder particles and reduces the melt pool distance. However, the microstructure of the steel can only be influenced to a limited extent.

The fracture behaviour of the printed steel shows a complex interplay of porosity, crystallographic grain orientation and hydrogen concentration. The combination of these effects influences the active failure mechanism during fracture. The elongation at fracture and the necking behaviour change, while the modulus of elasticity and tensile strength are minimally affected. For hydrogen-loaded RM specimens, a strain rate dependence of the failure mechanisms was demonstrated.

MM 16.9 Mon 18:30 Poster E

LPBF processed crack-free high-strength Al alloy — •Irena Paulin, Nejc Velikajne, Črtomir Donik, and Matjaž Godec — Institute of Metals and Technology, Lepi pot 11, Ljubljana, Slovenia

The ambitious goal of our research involves the development of a new high-strength Al alloy suitable for the AM process, which will facilitate the production of crack-free components combined with improved mechanical and corrosion properties. To achieve this goal, we prepared samples from commercially available AA7075 aluminium powder on a laboratory LBPF device. We changed various process parameters and optimized the production of simple samples in the form of 10x10x10 mm3 cubes, where we achieved the highest densities. Cracks were visible in all samples, regardless of the variety of process parameters used.

To avoid cracks, we process the samples at different temperatures of the preheated baseplate, where it turned out that higher temperatures do not have a favourable effect on the production of material without cracks. Surprisingly, lower preheating temperatures ensured better remelting in the material and thus less porosity in the material. In order to try to produce a material without cracks, in the next steps we started mixing AA7075 and AlSi12 powder, adding Si to the base material and thus reducing the difference in solidification temperature. Microstructural characterization showed that we successfully made a material without cracks.

MM 16.10 Mon 18:30 Poster E

PBF-LB of Soft Magnetic Fe-Based Metallic Glasses — •Felix Römer[1], Florian Spieckermann[1], Parthiban Ramasamy[2], and Jürgen Eckert[1,2] — [1]Montanuniversität Leoben, Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Leoben, Austria

Reducing the energy losses is a key requirement in the development of soft magnetic materials.

In recent years, interest has focused on nanocrystalline soft magnetic alloys, whose magnetic properties benefit from their chemical and structural variations at the nanoscale. Unfortunately, the nanocrystalline Fe- BMG's suffers from extreme embrittlement. Thus, they must be annealed in the final core geometry and handled very carefully.

The possibility of additive manufacturing of metallic glasses has drawn a lot of attention. This technique provides high heating and cooling rates, making it suitable for producing metallic glass parts with dimensions much bigger than their critical casting diameter. Besides the high heating and cooling rates, the layer-by-layer construction of the part results in a complex heat treatment of the preceding layers. Understanding the behavior of metallic glasses under these high rates and complex treatment is the key to printing dense, crack-free parts with suitable magnetic properties.

In the current study we show the effects of double scanning and random line strategy as well as preheating of the building platform on the microstructure, crack formation and thermal properties of KUAMET6B2 Fe72.6Si11.3B10.9Cr2.2C3.0 (at%).

MM 16.11 Mon 18:30 Poster E

Investigation of the Anisotropic Conductivity in Printed Nanosilver — •Lennart Schwan[1,2], Michael Feige[1], Laila Bondzio[2], Hütten Andreas[2], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Hochschule Bielefeld - University of Applied Sciences and Arts — [2]Thin Films & Physics of Nanostructures, Bielefeld University

3D printing is an emerging technology with a wide range of applications. The modern multi-material jetting process, such as that used in the Nano Dimension Dragonfly Pro LDM, makes it possible to print dielectric and conductive materials in a single process. In addition to printing flat structures such as printed circuit boards, three-dimensional structures such as antennas, coils or cooling elements can also be realized.

A special characteristic of the printed conductive material is the anisotropy of the electrical conductivity. Our investigation is dedicated to the origin of the anisotropy.

Investigations in the SEM show a direction-dependent crack structure. In order to investigate the influence of the cracks, we generate geometries from SEM images of the surface and simulate the current flow and the influence/impact on the effective conductivity using FEM. A further explanation results directly from the printing process, in which the surfaces are created from alternating offset printing lines. In order to investigate the influence of the resulting boundary layers on the anisotropic conductivity, we create additional boundary layers by manipulating the printing process.

MM 16.12 Mon 18:30 Poster E

Usability and Performance Analysis of 3D-Ink-Jet-Printed Load Cells with Resistive and Capacitive Strain Gauges — •Michael Feige, Lennart Schwan, and Sonja Schöning — Institute for Applied Materials Research (BIfAM), Hochschule Bielefeld - University of Applied Sciences and Arts, Bielefeld, Germany

Strain gauges can be used in a variety of different measurements e.g., to measure forces in manufacturing systems, to continuously monitor displacement of building structures. Furthermore, are they used in simple bathroom scales, kitchen scales and precision instruments with accuracies up to thousands of a gram. We utilize a 3D-Ink-Jet-Printer to manufacture flexible plastic devices with integrated strain gauges consisting of traces for resistive measurements or electrode arrays for capacitive measurements made of sintered silver ink. This additive manufacturing process provides a big advantage in scalability and flexibility over conventional methods and can avoid the necessity of bonding the strain gauges to a substrate adhesively. Printing measuring devices with dimensions of several millimeters up to several centimeters, an adaption to fulfill different geometric constraints e.g., due to housing or mounting, and fine tuning by thinning or thickening materials in particular areas is possible without great effort. Even more or less complex formations of multiple strain gauges combined in one device are feasible. We print different designs and examine them with regard to their sensitivity, hysteresis, non-reversible effects of stress and temperature stability.

MM 16.13 Mon 18:30 Poster E

Electrochemical study of Hydrogen Embrittlement in Al-Si coated stainless steels — •Neil Reon Mathias[1], Alisa Svirina[2], Sebastian Pentz[1], and Ferdinand Haider[1] — [1]Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg (Germany) — [2]Institute de Mécanique et Ingéniere, Université de Bordeaux (France)

There is a compelling business case for optimizing stainless steels for usage in hydrogen storage tanks. One method of reducing the penetration of hydrogen and accordingly the embrittlement of stainless steels is by coating it using the hot-dip process, which forms a layer of Al-Si on the surface to mitigate the embrittlement process. This study performs electrochemically controlled hydrogen permeation on different coated and uncoated stainless steels using a Devanathan-Stachurski cell to understand the nature of protection offered by these coatings. A set of commercial-grade austenitic, ferritic, duplex, and hot-dipped stainless steels are investigated for changes in their microstructure and fracture behaviour at room temperature. Evolution of trapped hydrogen is measured through thermal desorption spectroscopy to validate the electrochemical measurements. The hot-dip coating seems to reduce the hydrogen permeation considerably, thereby resulting in less hydrogen embrittlement compared to uncoated stainless steels. Microstructural changes indicate that the uncoated stainless steels show greater degree of intergranular fracture compared to the coated stainless steels. Tensile test results demonstrate the increased elongation of coated stainless steels in comparison to their uncoated counterparts.

MM 16.14 Mon 18:30 Poster E

Effect of Ilmenite reduction pathway on TiFe hydrogen storage properties obtained by Sieverts apparatus measurement — •Matthieu Ramond[1,2], Alexander Haack[1,2], Gabby Hunter-Smith[3], Mohammad Zarar[3], Karl Shaffer[4], Karl Dahm[5], Chris Bumby[3], Paul Jerabek[2], Thomas Klassen[2,6], Nigel Lucas[1,7], and Claudio Pistidda[2] — [1]University of Otago, Department of Chemistry, Dunedin, New Zealand — [2]Helmholtz-Zentrum Hereon, Institute of Hydrogen Technology, Geesthacht, Germany — [3]Victoria University of Wellington, Paihau-Robinson Research Institute, Wellington, New Zealand — [4]Victoria University of Wellington, Ferrier Research Institute, Wellington, New-Zealand — [5]Callaghan innovation, Lower Hutt, New Zealand — [6]Helmut Schmidt University, Faculty of Mechanical Engineering, Institute of Materials Science, Hamburg, Germany — [7]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

New Zealand has large quantities of naturally occurring ilmenite (TiFeO3) ore. Samples of this easily available oxide were thermally reduced to a titanium-iron alloy under a variety of experimental conditions, e.g., temperatures, durations, and grind sizes at Victoria University of Wellington. After thermal activation under dynamic vacuum, hydrogen adsorption and desorption cycles were measured. The hydrogen uptake properties of the alloys can be determined using a specially-built Sieverts apparatus. The gravimetric storage and kinetics of the samples were evaluated by numerical fitting, enabling these properties to be linked to the reduction process.

MM 16.15 Mon 18:30 Poster E

Experimental and computational study of the effects of metal-based additives on the dehydrogenation process of the 2NaBH4 + MgH2 system — •Yuanyuan Shang[1], Archa Santhosh[1], Ou Jin[2], Fahim Karimi[1], Thi Thu Le[1], Dorothée Vinga Szabó[2], Stefan Wagner[2], Christian Kübel[2], Paul Jerabek[1], Astrid Pundt[2], and Claudio Pistidda[1] — [1]Department of Materials Design, Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, 76131, Karlsruhe, Germany

We report a systematic investigation of the effect that selected metal-based additives have on the dehydrogenation properties of the reactive hydride composite (RHC) model system 2NaBH4+MgH2. Compared to the pristine system, the material doped with 3TiCl3*AlCl3 exhibits superior dehydrogenation kinetics. The addition of 3TiCl3*AlCl3 alters the controlling mechanism of the second dehydrogenation step making it change from a two-dimensional interface-controlled process to a two-dimensional nucleation and growth controlled process. Nanostructured metal-based phases, such as TiB2/AlB2 particles, appear to act as heterogeneous nucleation sites for MgB2. For this reason, the properties of the TiB2/MgB2 interface were investigated by first-principles calculations utilizing density functional theory (DFT).

MM 16.16 Mon 18:30 Poster E

Electrochemical loading of magnesium-palladium thin films in KOH — •Giorgia Guardi[1], Angelina Sarapulova[1], Sonia Dsoke[1], Stefan Wagner[1], Luca Pasquini[2], and Astrid Pundt[1] — [1]Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT), Germany — [2]Department of Physics and Astronomy, University of Bologna, Italy

The magnesium-hydrogen system is of interest for hydrogen storage applications due to the high hydrogen density (7.6 wt.%) achievable in magnesium hydride (MgH_2). There are however drawbacks, such as the slow diffusion of hydrogen in MgH2. This drawback can be overcome by using nanostructured materials such as thin films, where the hydrogen diffusion coefficient increases due to the high concentration of grain boundaries. This leads to faster hydride formation.

Hydrogen charging of magnesium by means of electrochemistry is challenging due to its high corrosion tendency. In this work we show how the electrochemical hydrogen loading of Mg-Pd thin films can be optimised in KOH. It is revealed how the loading potential influences the hydride formation mechanism, and how its optimal value can be found by performing cyclic voltammetry and hydrogenography experiments.

MM 16.17 Mon 18:30 Poster E

Measurement of Tritium Content with a novel Detector System — •Joris Müller, Christoph Kirchlechner, and Xufei Fang — IAM, KIT, Karlsruhe, Germany

Hydrogen Embrittlement (HE) and the involved mechanisms are still being heatedly debated today. It yet remains a challenge to quantify the embrittlement due to the difficulty in precisely detecting hydrogen via most existing methods, while ones with high precision (e.g., Atom Probe Tomography) are limited to very local areas under special conditions (e.g., deuterium charging). Here, we present a concept of using a high-resolution, spatially-resolving direct electron detector, akin to a radiation camera, by taking advantage of using the radioactive hydrogen isotope tritium. After exposing samples to tritium, the β-decay can then be detected to enable a positionally accurate depiction of its position in the crystal lattice. One proposed concept makes use of a parallel-hole collimator for direction-wise filtering in order to achieve a parallel projection image in combination with a stacked microchannel plate (MCP) array for amplification, followed by a phosphorescent screen and high-resolution camera functioning as an electron to photon and finally signal converter. A setup like this will, in an ideal case, enable in situ real-time tracking of tritium during micromechanical tests, allow quantification of the mechanical properties with the presence of hydrogen in the materials' defects (e.g., grain boundaries), and help to gain a better understanding of the hydrogen embrittlement mechanisms in metals.

MM 16.18 Mon 18:30 Poster E

Microstructural Influencing Factors on Susceptibility of High Strength Steels against Hydrogen Embrittlement — Ingrit Sisilia Rosari Nurak[1] and •Michael Brilz[2] — [1]KIT, Karlsruhe (Gebäude 30.25, Raum 217) — [2]MPA IfW Darmstadt

This thesis aims to conduct a materials science-based analysis of the relationship between microstructural, chemical, and fracture mechanical factors and the susceptibility to hydrogen embrittlement. For this purpose, metallographic and fracture mechanical examinations are done via VVT tests. To analyze the correlation between microstructural and fracture mechanical parameters, three materials with different microstructures are loaded with a constant HCl concentration and then strained, while for the investigation of the correlation between chemical and fracture mechanical parameters, identical samples are loaded with different HCl concentrations and then strained. An important microstructural influencing factor for quenched and tempered steels is the grain size of former austenite grains.

MM 17: Poster Ib

Time: Monday 18:30–20:30 Location: Poster F

MM 17.1 Mon 18:30 Poster F

Implementation of Experimental Results in an Ontology of Magnetocaloric Materials Research — Simon Bekemeier[1], Moritz Blum[2], Luana Caron[3,4], Philipp Cimiano[2], Basil Ell[2], Inga Ennen[3], Michael Feige[1], Maik Gaerner[3], Thomas Hilbig[1], Andreas Hütten[3], Günter Reiss[3], Tapas Samanta[3], Sonja Schöning[1], Christian Schröder[1,3], Lennart Schwan[1,3], and •Martin Wortmann[3] — [1]University of Applied Sciences and Arts, Bielefeld, Germany — [2]Faculty of Technology and CITEC, Bielefeld University, Bielefeld, Germany — [3]Faculty of Physics, Bielefeld University, Bielefeld, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Magnetic refrigeration based on the magnetocaloric effect is an environmentally friendly alternative to compression based cooling. The cooling effect is based on heat release or uptake during magnetic phase-transitions of a magnetocaloric material. The decades-long search for alloys suitable for mass application could be made much more efficient by digitizing the scientific process chain. The project DiProMag seeks to digitalize the process chain from theory, simulation and experiment to prototypical applications in an ontology. Here, we show how experimental results are implemented in a hierarchical ontology. Various Heusler alloys have been investigated as thin films, nanostructures, and bulk material. Different approaches have been developed for these materials to be integrated into functional prototypes. The goal is to standardize data evaluation and reporting to make it more accessible and comparable across different fields within the community.

MM 17.2 Mon 18:30 Poster F

Electronic structure fingerprints of nickel-cobalt-manganese oxide from high-throughput ab initio calculations — •Timo Reents[1], Daniel Duarte-Ruiz[1], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg — [2]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin

Nickel-cobalt-manganese (NCM) oxides are established cathode materials for energy storage. Their structural complexity outlines the challenges of modelling these systems in realistic stoichiometries and compositions. Ab initio methods embedded in automatized workflows are particularly suited to address this task as they provide a tool to efficiently perform quantum-mechanical calculations on multiple structures. In this work, we model possible candidates by exchanging the transition metals atoms of $\mathrm{LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2}$ to adjust their concentration. This offers a handle to tune the structural and electronic properties of the materials to match the desired composition. By exploiting data-driven methods on top of the computed projected density of states (PDOS), we group the results into clusters and propose a scheme to relate structural properties to PDOS fingerprints. The insight gained into the distribution of different oxidation states and the local structural arrangements is utilized to interpret x-ray absorption data from synchrotron measurements. The good agreement obtained in this procedure confirms the validity of the adopted computational approach and offers excellent perspectives for their application to other classes of technologically relevant compounds.

MM 17.3 Mon 18:30 Poster F

From ab-inito to experiments: A Python workflow for constructing neuroevolution potentials — •Eric Lindgren[1], Adam Jackson[2], Zheyong Fan[3], Christian Müller[4], Jan Swenson[1], Thomas Holm-Rod[5], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, United Kingdom — [3]College of Physical Science and Technology, Bohai University, Jinzhou, People's Republic of China — [4]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden — [5]ESS Data Management and Software Center, Copenhagen, Denmark

Neuroevolution potentials, NEPs, as implemented in the GPUMD package are a highly accurate and computationally efficient type of machine-learned interaction potentials, enabling large scale MD simulations with system sizes up to millions of atoms with ab-initio level accuracy. Here, we present a Python workflow for constructing and sampling NEPs using the 'calorine' package, and how the resulting trajectories can be analysed with the 'dynasor' package to predict observables from scattering experiments. We focus on our recent work on crystalline benzene as an example system, but the approach is readily extendable to other systems.

MM 17.4 Mon 18:30 Poster F

Interoperable data workflows: A case study on non-vdW 2D systems — •Mani Lokamani[1], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden — [4]Duke University, Durham, USA

Interoperability and compatibility of research data and workflows from different, complementary simulation ecosystems are the key enabler for data-driven materials design. Two such simulation environments are (i) AFLOW [1], with its standardized workflows that generate huge amounts of compatible data, and (ii) AiiDA [2], which provides a customizable workflow that is often employed for dedicated projects by interfacing with several different *ab initio* programs.

Here, we aim at exploring the transferability and interoperability of data and workflows between the two frameworks. As a case study, we focus on the emerging class of non-van der Waals 2D materials, which have attracted considerable interest in recent years due to their unique electronic and magnetic properties [3]. In the first step, metadata are retrieved using AFLOW. Then, the extracted parameters are adapted with an AiiDA-plugin for accurate electronic structure calculations using the full-potential all-electron code FLEUR [4] within AiiDA.

We acknowledge support from the Helmholtz HIDA trainee network.

[1] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).

[2] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).

[3] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).

[4] The FLEUR project: https://www.flapw.de.

MM 17.5 Mon 18:30 Poster F

Investigating phonons in superconducting Lanthanum Hydride using ab initio methods accelerated by machine learning potentials. — •Abhishek Raghav[1], Kousuke Nakano[2], and Michele Casula[1] — [1]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France — [2]Center for Basic Research on Materials, National Institute for Materials Science (NIMS), Tsukuba, Japan

Hydrogen rich materials with calthrate structures are an important class of superconducting materials. Lanthanum hydride ($\mathrm{LaH_{10}}$) is one such material, demonstrated to show superconductivity at 250 K and 170 GPa.

Phonon spectrum and electron-phonon coupling are important ingredients used to predict superconductivity, being of BCS type. However, computing accurate phonons for hydrogen calthrate materials requires including anharmonicity due to nuclear quantum effects. In this work, we use the path integral molecular dynamics (PIMD) formalism to compute accurate anharmonic phonons. It is observed that, phonons for $\mathrm{LaH_{10}}$ ($\mathrm{Fm\bar{3}m}$ phase), as predicted by PIMD are dynamically stable over the experimentally relevant pressure range, in contrast with the harmonic phonons. We also use the energies and forces computed during PIMD to train a machine learning potential (MLP) for $\mathrm{LaH_{10}}$ using operator quantum machine learning. This MLP is then used to drive simulations with larger supercells, to compute phonons efficiently and accurately.

MM 17.6 Mon 18:30 Poster F

Machine-learning based optimization of hafnium-zirconium oxide compositions for stable ferroelectric applications in non-volatile memories — •Arunima Singh and Patrick Rinke — Department of Applied Physics, Aalto University

CMOS-compatible hafnium dioxide ($\mathrm{HfO_2}$) based ferroelectrics (FE) are widely studied for use in non-volatile memories. Zr-doping of $\mathrm{HfO_2}$ i.e. hafnium-zirconium oxide (HZO) has further improved the FE properties. However, the optimum HZO structure and stoichiometry ($\mathrm{Hf_{1-x}Zr_xO_2}$) still needs to be found. In this work, we used machine-learning assisted density-functional theory (DFT) calculations [1] to map out and characterize $\mathrm{Hf_{1-x}Zr_xO_2}$ and to find optimal configurations in the materials space. We built an initial dataset of $\mathrm{Hf_{1-x}Zr_xO_2}$

structures and their corresponding single point DFT energies. A kernel ridge regression (KRR) machine learning model is trained on this dataset and then further refined with active learning that picks appropriate structures from DFT relaxation trajectories. The atomic structures are represented in the vector form with many-body tensor representation (MBTR). With the refined KRR model, we explored the full HZO configuration space and optimized for structural stability and FE (also calculated with DFT).
[1] J. Laakso, M. Todorović, J. Li, G. X. Zhang & P. Rinke, *Compositional engineering of perovskites with machine learning*, Physical Review Materials, 6(11), 113801, (2022).

MM 17.7 Mon 18:30 Poster F

Computational Workflow for Defect Calculations for Solar Cell Applications — •Lotte Kortstee and Ivano Eligio Castelli — Department of Energy Conversion and Storage, Technical University of Denmark, Anker Engelundsvej 411, DK 2800 Kgs. Lyngby, Denmark

To aid the discovery of new functional materials and encourage the shift towards sustainable energy sources, the employment of computational tools is essential. A workflow-centered approach is used to study defects in perovskite materials that serve as an indicator for solar cell efficiency.

Using the framework of Density Functional Theory, a workflow is created using the Pydefect package and Atomistic Simulation Environment (ASE). The workflow is used to generate a chemical phase diagram, that identifies the chemical potentials under which the target material is stable. From there, defect calculations are performed on vacancies, interstitials and antisites of varying charge. Moreover, the band-structure and density of states of the compounds are determined to locate charge transition levels in relation to the band gap edges. Using Climbing Image Nudged Elastic Band (CINEB), the kinetics of point defects in the structure can be assessed and related to the formation energy of point defects.

We have applied this workflow to discover perovskites for solar cell applications, focusing on gold-containing tetragonal double perovskites. The properties of these materials are being investigated experimentally at our partner university.

MM 17.8 Mon 18:30 Poster F

Modification of bimetallic sulfide anodes for sodium ion storage — •Zidong Wang — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to their high specific capacity and long cycle life, bimetallic sulfides are the preferred choice of researchers as anodes in sodium-ion batteries (SIBs). However, studies indicate that this class of materials often requires expensive elements such as Co, Sb, Sn, etc., and their performance is insufficient with the use of inexpensive Fe, V alone. Therefore, there is a need to explore the relationship between metal cations and anode performance so that the requirements of cost reduction and performance enhancement can be met simultaneously. In this work, a series of partially re-placed sulfides with different cation ratios have been prepared by hydrothermal method followed by heat treatment. By partially replacing Co in NiCo sulfides, all samples show improved capacity and stability over the original NiCo sulfides. As a result, the metal elements have different oxidation states, which leads to a higher capacity through their synergistic effects on each other.

MM 17.9 Mon 18:30 Poster F

Machine-Learned Molecular Dynamics Simulations of Doping Effects in Sodium Ion Conductors — •Namita Krishnan, Takeru Miyagawa, Manuel Grumet, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

Na-based solid-state ion conductors (SSICs) are set to revolutionize next-generation batteries due to low cost and availability relative to their lithium-based counterparts. Still, Na-based SSICs have considerably lower ionic conductivities relative to conventional electrolytes, a factor that hampers their commercialization. Doping is one way to mitigate this disadvantage by maximizing ion conduction pathways without compromising the host lattice's structural integrity [1,2]. A sophisticated choice of dopant elements requires a deep understanding of the interplay between the dopants, mobile Na ions, and the host lattice. Ab initio molecular dynamics (AIMD) simulations offer atomistic insights into the lattice dynamics of doped SSICs but are computationally tedious. Therefore, we investigate the accuracy of machine-learned molecular dynamics (MLMD) for vibrational properties and diffusion coefficients of doped sodium ion conductors compared to AIMD simulations. We then apply the ML-generated force fields to investigate the effect of homovalent and aliovalent doping in Na_3SbS_4.

References [1] T. Fuchs, et al. ACS Energy Lett., 2019, 5, 1, 146-151. [2] R. Jalem, et al. J. Mater. Chem. A, 2022 10, 5, 2235-2248.

MM 17.10 Mon 18:30 Poster F

Disorder in electronic properties of 2D and 3D perovskites on the nanoscale — •Andrii Shcherbakov[1,2], Darwin Korte[1], Shangpu Liu[1,2], Markus Heindl[1,2], Stanislav Bodnar[1,2], Jonathan Zerhoch[1,2], and Felix Deschler[1] — [1]Physikalisch-Chemisches Institut Universität Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg — [2]Walter Schottky Institut Technische Universität München,Am Coulombwall 4, 85748 Garching bei München

Because of outstanding semiconducting properties like high quantum yield, tuneability, and potential to form quantum confined systems, organic-inorganic hybrid perovskites have proved themselves as attractive candidates for various optoelectronic applications, including efficient photodetectors, light emitting diodes and solar cells. Local electronic properties affected by the disorder caused by strain, defects, and differences in confinement have a direct influence on the optical properties and the device's performance. By studying the types of such inhomogeneities, their influence on key semiconducting properties, and their dependence on the fabrication process, we can adjust the latter to achieve the best performances. Here, we start investigating our test materials with the means of confocal (circular) photoluminescence spectroscopy, allowing to study disorder on the microscale. By further employing nearfield nanoscopy, we achieve spatially resolved material response with a resolution below the diffraction limit. Finally, we find a correlation between the fabrication conditions and the disorder, suggesting us ways of increasing the performance of the product material.

MM 17.11 Mon 18:30 Poster F

Functional properties of aerosol deposited thick lead-free piezoelectric ceramic films — •Michel Kuhfuss[1], Juliana G. Maier[1], Alexander Martin[2], Ken-ichi Kakimoto[2], Neamul H. Khansur[1], and Kyle G. Webber[1] — [1]Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany — [2]Department of Life Science and Applied Chemistry, Nagoya Institute of Technology, Nagoya, Japan

The powder aerosol deposition (AD) method is a technique to deposit thick, dense ceramic films through room temperature impact consolidation (RTIC). AD is a promising method for applications such as piezoelectric energy harvesting due to being cost-effective and rapid. However, deposited films differ from bulk ceramics due to internal stress, RTIC-induced defects, and nanometer-range grain size. Therefore, the impact on the functional properties of different lead-free piezoelectric materials is investigated with electromechanical measurements. They reveal a direct connection between the piezoelectric response and the grain size. For comparison, the grain size dependence is analyzed with in situ electric field-dependent synchrotron X-ray diffraction. Further, processing methods such as annealing are conducted to enhance the properties of the deposited films.

MM 17.12 Mon 18:30 Poster F

interaction of hydrogen with local heterogeneities: correlating simulations and experiments — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]IMPRS SusMet, Max-Planck-Institut für Eisenforschung GmbH — [2]LWT, Ruhr-Universität Bochum — [3]ICAMS, Ruhr-Universität Bochum

The term "hydrogen embrittlement" (HE) refers to multiple phenomena related to the detrimental effects of hydrogen in metallic materials. The most effective approach to mitigate HE involves reducing hydrogen diffusion within microstructures, requiring a thorough understanding of the impact of local heterogeneities at various length scales. Advanced experimental and computational methods exist for this purpose, but they are usually applied to samples or models, of rather different complexity, and thus it is always a question of how to compare and combine their results. In this study, ab initio density functional theory calculations were used to calculate the diffusion barrier of hydrogen under the influence of different local chemistry. Simultaneously, differently alloyed Fe-based alloys are produced on a laboratory scale, and subjected to various heat treatments to achieve microstructures representing different local microstructural characteristics, for which atomistic simulation models shall be set up as well. This poster shows the first insights on how to combine more effectively simulation and experimental methods to shed light on how inevitable heterogeneities impact the hydrogen behavior in iron and steel.

MM 17.13 Mon 18:30 Poster F

Mechanochemical Pathway to Nickel — •Jikai Ye[1], Christian H. Liebscher[2], and Michael Felderhoff[1] — [1]Max-Planck-Institut für Kohlenforschung, Department of Heterogeneous Catalysis, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Metal oxide reduction is the key step to metal production in the process of both primary and secondary metal production. However, traditional methods usually correlate with high energy consumption from heating and CO_2 emission from carbonaceous reductants. Mechanochemistry describes certain reactions that can happen with the help of mechanical forces under much milder conditions, which could enable more sustainable pathways for metal productions. In this work, the possibility of reducing metal oxides at room temperature under hydrogen with ball-milling is confirmed, using NiO as an example. In a planetary ball-mill batch system under hydrogen pressure, NiO could be partially reduced, reaching an equilibrium state upon generation of water vapor. Further, with the help of a home-built gas-flow shaker-mill system, generated water from the reaction between NiO and hydrogen could be removed continuously. A much higher reduction degree could therefore be achieved. With mild heating (<100 °C) during milling, reaction rate could be significantly increased benefiting from faster desorption of water. With this method, Ni nanoparticles were synthesized. Primitive tests also confirm that the as-synthesized Ni nanoparticles exhibit high catalytic activity over hydrogenation.

MM 17.14 Mon 18:30 Poster F

Raman Spectroscopy and Photoluminescence Studies on Recyclate-based MgO-C Composites — •Julia Richter[1], Cameliu Himcinschi[1], Mahnaz Mehdizadehlima[2], Serhii Yaroshevskyi[3], Till Manon Jannis Stadtmüller[3], and Jens Kortus[1] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Straße 23, D-09599 Freiberg, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Straße 5, D-09599 Freiberg, Germany — [3]Institute of Ceramics, Refractories and Composites, TU Bergakademie Freiberg, Agricolastraße 17, D-09599 Freiberg, Germany

Re-usage, recycling and upcycling of MgO-C refractories are crucial for resource efficiency. Antioxidants used as additives as well as metal and slag residuals reduce the quality of the recycled raw material. Environmentally friendly binders, e.g. lignin-collagen systems, are supposed to replace commonly used binders, such as pitch and resin, in order to save resources and to lower CO2 emissions as well as harmful effects on the environment. In this work, Raman and photoluminescence (PL) spectroscopy as sensitive, non-destructive, non-contact methods are applied to detect impurities and to characterize the carbon structures, in particular carbon cluster size, depending on the binder system in the refractory material.

On the other hand, MgO-C recyclate-based anode materials for application in the extraction of aluminum by fused-salt electrolysis are investigated by Raman and PL and their spectra compared with those of pure materials.

MM 17.15 Mon 18:30 Poster F

Optothermal analysis of Indium thiospinels — •André Strassheim[1], Cameliu Himcinschi[1], Ayberk Özden[2], Esteban Zuñiga-Puelles[3], Roman Gumeniuk[3], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Electronic and Sensor Materials, D-09599 Freiberg, Germany — [3]TU Bergakademie Freiberg, Institute of Experimental Physics, D-09599 Freiberg, Germany

The temperature dependence of thermal conductivities of crystalline Indium thiospinels were characterized by optothermal Raman spectroscopy, a contactless method that can be used for small sample volumes. The obtained values are in fair agreement with those obtained from conventional laser flash analysis and thus, validates the employed technique. The temperature-dependent thermal conductivity of one Indium thiospinel sample was measured from 100 K to 343 K in steps of 50 K and ranged from 5.1 $\frac{W}{mK}$ to 1.7 $\frac{W}{mK}$.

Furthermore, a reversible β ($I4_1/amd$) to α ($Fd\bar{3}m$) phase transition was identified through temperature-dependent Raman spectroscopy. It was observed to be reversible and to occur between 440 K and 450 K.

In conclusion, this study suggests that optothermal Raman spectroscopy emerges as a valuable technique for probing the thermal properties of materials, particularly in cases where material volume is limited and when dealing with arbitrary shapes.

MM 17.16 Mon 18:30 Poster F

Direct visualization of electric current induced dipoles of atomic impurities — •Yaowu Liu[1,2], Zichun Zhang[1], Sidan Chen[1], Shengnan Xu[1], Lichen Ji[1], Wei Chen[1], Xinyu Zhou[1], Jiaxin Luo[1], Xiaopeng Hu[1], Wenhui Duan[1], Xi Chen[1], Qikun Xue[1,3,4,5], and Shuaihua Ji[1,5] — [1]State Key Laboratory of Low-Dimensional Quantum Physics, Department of physics, Tsinghua University, Beijing 100084, China — [2]Center for Quantum Nanoscience, (IBS), Seoul 30760, Republic of Korea — [3]Beijing Academy of Quantum Information Sciences, Beijing 100193, China — [4]Department of Physics, Southern University of Science and Technology, Shenzhen 518055, China — [5]Frontier Science Center for Quantum Information, Beijing 100084, China

Learning electron scattering around atomic impurities is vital for comprehending the basic electronic transport phenomena. Despite many efforts in the past several decades, atomic scale transport around single point-like impurities has yet been achieved. Here, we report the direct visualization of the electric current induced dipoles around single atomic impurities in epitaxial bilayer graphene [arXiv:2309.01182]. We find the directions of these dipoles are determined by the charge polarity of the impurities, revealing the direct evidence for the existence of the carrier density modulation effect proposed by Landauer in 1976 [Phys.Rev.B 14,1474 (1976)]. Furthermore, by in situ tuning local current directions, these dipoles are redirected correspondingly. Our work paves the way to explore the quantum transport phenomena at single atomic impurity level.

MM 17.17 Mon 18:30 Poster F

Tuning thermal and ionic transport properties of sodium superionic conductors for advanced energy storage: insights from molecular dynamics simulations — •Insa de Vries, Freya Hallfarth, and Nikos Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

In the pursuit of resource-efficient and sustainable energy storage solutions, sodium-based electrolytes increasingly attract attention as a compelling choice for energy materials. Notably, sodium superionic conductor (NASICON)-type lattices have demonstrated promising ionic conductivities, positioning them as viable candidates for battery applications [1]. However, the development of a secure battery design necessitates, in addition, a comprehensive understanding of thermal conduction properties to mitigate localized heat accumulation during battery operation.

We conducted classical molecular dynamics simulations of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ class of compounds for various stoichiometries (x=2, 2.4, and 2.8) using an interionic potential derived before [2]. Structural order of the Si and P cations is found to enhance diffusion. Its influence on thermal conductivity, assessed by a Green-Kubo approach, is discussed. A decrease in thermal conductivity is observed upon suppression of sodium ion diffusion.

[1] C. Zhao et al., Adv. Energy Mater. 2018, 8, 1703012
[2] P. Kumar & S. Yashonath, J. Am. Chem. Soc. 2002, 124, 3828

MM 17.18 Mon 18:30 Poster F

Ab-initio simulation of electronic transport in amorphous phase change materials — •Nils Holle[1], Sebastian Walfort[1], Riccardo Mazzarello[2], and Martin Salinga[1] — [1]University of Münster, Institute of Materials Physics, 48149 Münster — [2]Sapienza Università di Roma, Department of Physics, I-00185 Roma

As the global demand for computing resources continues to grow, the need to improve the energy efficiency of computing hardware is becoming increasingly important. The miniaturisation of electronic devices based on phase change materials (PCMs) has been shown to enable significant reductions in power consumption. These materials exist in both a crystalline and an amorphous configuration and exhibit a strong electrical contrast between these configurations. This makes them interesting for a wide range of applications, such as data storage and neuromorphic computing. A detailed understanding of electronic transport is a crucial step towards designing a new generation of energy-efficient functional electronic devices. However, despite many years of research, electronic transport in amorphous PCMs is still not fully understood, as it is complicated by disorder and its consequences, such as structural inhomogeneity. We study transport in a single-element PCM that is strongly confined between adjacent electrodes. The combination of density functional theory and non-equilibrium Green's functions provides the ideal means to gain ab-initio insight into electronic structure and transport on an atomistic scale. Based on our observations, we propose a new physical picture where conductivity is governed by local variations in Peierls-like distortions.

MM 17.19 Mon 18:30 Poster F

Accurate ab initio vacancy properties in concentrated Mo-Ta alloys from machine-learning potentials — •Xiang Xu[1,3], Xi Zhang[1], Sergiy Divinski[2], and Blazej Grabowski[1] — [1]Institute for Materials Science, University of Stuttgart, Germany — [2]Institute for Materials Physics, University of Münster, Germany — [3]Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart, Germany

We utilize a bespoke machine-learning interatomic potential, i.e., moment tensor potential (MTP) to predict thermodynamic properties of vacancy formation. The highly optimized MTP is trained with snapshots from ab initio molecular dynamics simulations within the active learning framework. For the vacancy formation energy, we utilize the special quasi-random structure approach in conjunction with a statistical analysis, from which temperature-dependent formation Gibbs energies as well as averaged atomic environments can be extracted. We show that the temperature-dependent vacancy formation Gibbs energy due to ”configurational excitations” has a negative entropy contribution while thermal vibrations provide a positive entropy. The local chemical environment effect and general trends are also analyzed.

MM 17.20 Mon 18:30 Poster F

Machine learning approach to obtaining the scattering self-energy from transmission calculations — •Fabian Engelke, Markus Kremer, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität, Institute for Theoretical Physics, Gießen, Germany

Aiming to assist the development of nanoscale electronic devices, we contribute to developing ab initio transport calculations. This work is particularly concerned with treating phase-breaking scattering events due to the electron-phonon interaction. In the Keldysh formulation of the non-equilibrium Green*s function formalism, as implemented in a Korringa-Kohn-Rostoker electronic structure code, those scattering events are characterized by an additional self-energy. Even though it is possible to estimate the self-energy, those calculations involve many approximations, such as k-vector averaging and Wannier-function interpolation of band structures.

Introducing a new way to calculate the self-energy, we train a deep neural network based on conventionally calculated self-energies and transmission calculation results from the Keldysh formulation. We then use this neural network to map transmission results based on the molecular dynamics Landauer approach back to the self-energy.

MM 17.21 Mon 18:30 Poster F

Multi-scale modeling of heat conduction in filled polymer composites — •Oliver Roser[1,2], Andreas Griesinger[3], and Othmar Marti[2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Institute of Experimental Physics, Ulm University — [3]Baden-Wuerttemberg Cooperative State University (DHBW), Stuttgart

When polymers are modified with granular fillers to increase thermal conductivity, the simultaneous viscosity increase of the composite often limits the allowable filler concentration and thus the achievable thermal conductivity. If fillers from several size classes are smartly combined, the viscosity increase can be mediated and the allowable filler concentration increased. The result is a complex material whose microstructure extends over several orders of magnitude. The largest particles used may be thousands of times larger than the smallest. For a detailed simulative analysis of the heat transport phenomena in such materials, we have designed a new multi-step homogenization approach. This approach allows us to take into account the filler structure in all size scales and to calculate the achievable thermal conductivity as a function of the filler composition. Starting with the heat transfer from the smallest filler particles into the polymer up to the large spatial heat paths between the largest filler particles, all effects are taken into account. We present our multi-step homogenization approach, experimental validation, and the results of computational studies on the optimal composition of filler blends.

MM 18: Topical Talk: Dierk Raabe

Time: Tuesday 9:30–10:00 Location: C 130

Topical Talk MM 18.1 Tue 9:30 C 130

Transport and phase transformations in sustainable hydrogen-based steel production — •Dierk Raabe, Yan Ma, Isnaldi Souza Filho, and Özge Özgün — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

Steelmaking causes 8% of all global greenhouse gas emissions, qualifying it as biggest single cause of global warming, due to the use of fossil carbon as reductant [1,2]. Mitigation strategies pursue the replacement of fossil carbon carriers by sustainably produced hydrogen and / or electrons. We presents progress in understanding the mechanisms of hydrogen-based direct reduction and plasma reduction of iron oxides and explain how metallization and kinetics depend on mass transport kinetics, nucleation and growth phenomena, chemical and stress partitioning, oxide chemistry and microstructure, porosity, plasticity, damage and fracture effects associated with the phase transformation phenomena occurring during reduction [3,4].

1. Raabe, D., Tasan, C. C. & Olivetti, E. A. Strategies for improving the sustainability of structural metals. Nature 575, 64-74 (2019).
2. Raabe, D. The Materials Science behind Sustainable Metals and Alloys. Chem. Rev. 123, 2436-2608 (2023).
3. Kim, S. H. et al. Influence of microstructure and atomic-scale chemistry on the direct reduction of iron ore with hydrogen at 700°C. Acta Mater. 212, 116933 (2021).
4. Souza Filho, I. R. et al. Green steel at its crossroads: Hybrid hydrogen-based reduction of iron ores. J. Clean. Prod. 340, 130805 (2022).

MM 19: Topical Session: Hydrogen in Materials: from Storage to Embrittlement II

Time: Tuesday 10:15–11:30 Location: C 130

Topical Talk MM 19.1 Tue 10:15 C 130

Hydrogen-Induced Fracture Behavior in Cr-Mo Low Alloy Steel: In-situ ETEM Insights on Crack Propagation — •Lin Tian[1], Masanobu Kubota[2], Petros Sofronis[2,3], Reiner Kirchheim[1,2,4], and Cynthia A. Volkert[1,2,5] — [1]Institute of Materials Physics, University of Göttingen, Göttingen, Germany — [2]International Institute for Carbon Neutral Energy Research, Kyushu University, Fukuoka Japan — [3]Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, USA — [4]Max-Planck-Institute for Iron Research, Duesseldorf, Germany — [5]The International Center for Advanced Studies of Energy Conversion (ICASEC), University of Göttingen, Göttingen, Germany

Taking advantage of an in-situ fracture test method inside an environmental transmission electron microscope (ETEM), the fracture behavior of a Cr-Mo low alloy steel is examined. Through controlled gas environments, we compared the fracture behavior of samples in vacuum and in hydrogen gas. In vacuum, the sample fractures by void nucleation and coalescence showing typical ductile fracture behavior. It is found that the ferrite matrix is the major void initiation site due to the low stress triaxiality in the thin sample. However, in the presence of hydrogen gas in the TEM chamber, clear evidence of hydrogen embrittlement is observed. The crack tip in hydrogen gas remains sharp and propagates by the formation and linking up of staircase-shape micro-cracks, without much associated plasticity. We will discuss possible contributions to embrittlement from the effect of hydrogen on (i) dislocation formation and mobility, and (ii) lattice decohesion.

MM 19.2 Tue 10:45 C 130

Microstructure-based modeling of fatigue damage of ferritic steel in hydrogen environments using crystal-plasticity-FEM simulation — •Alexandra Stark[1], Wolfgang Verestek[1], Petra Sonnweber-Ribic[1], and Christian Elsässer[2] — [1]Robert Bosch GmbH, CR, Renningen — [2]Fraunhofer IWM, 79108 Freiburg

Hydrogen Embrittlement (HE) of ferritic steels is a long and well-known phenomenon. Depending on its environment the material may be prone to a premature mechanical failure. In real world service, steel components are frequently exposed to cyclic loading. Therefore, with increasing relevance of hydrogen-related technologies, handling the influence of hydrogen on the fatigue behavior of steel is of growing interest.In the complex phenomenon of metal fatigue, one of the main factors that determine the lifetime is attributed to the microstructure of the metal. A well established approach to describe microstructural influences on the mechanical behavior of metals is the crystal plasticity (CP) theory [1]. CP finite element methods (CP-FEM) are useful to investigate fatigue damage in the material by a microstructure-sensitive modeling. In the present work, a diffusion coupled crystal plasticity model is used to investigate the influence of hydrogen on the fatigue behavior of a ferritic steel. Within this model the mechanical properties of the material are characterized by local hydrogen concentrations based on proposed HE-failure mechanisms. The study addresses the impact of environmental conditions and internal hydrogen concentrations on HE and investigates the influence on the prediction of fatigue damage. [1] F. Roters et al. Acta mater 58.4 (2010): 1152-1211

MM 19.3 Tue 11:00 C 130

Effect of retained austenite volume fraction on the hydrogen uptake and hydrogen embrittlement susceptibility of high-strength steels. — •Eric A.K. Fangnon and Yuriy Yagodzinskyy — Department of Mechanical Engineering, School of Engineering, Aalto University, P.O Box 11000, FI-00076, Espoo, Finland

Retained austenite (RA) is known for playing a dual role in the way hydrogen interacts with steels affecting their resistance or susceptibility to HE. In this study, we investigate the performance of five distinct high-strength steels with varying volume fractions of RA (0 - 35%) obtained from different alloying and heat-treatment processes. Electrochemical hydrogen charging under monotonic and cyclic loading modes was used to evaluate the steel's performance in hydrogenated conditions. In addition, the effect of RA on hydrogen uptake and phase transformation under load was investigated by thermal desorption spectroscopy, X-ray diffraction, and electron backscatter diffraction analysis. The Results show that there is a threshold at which the benefits of RA exist. After which the steels manifest severe susceptibility to HE as a function of RA volume fraction Via intergranular fracture modes for steels with higher contents of RA. Different hydrogen uptake and trapping were observed for the steels as a function of RA volume fraction, Load magnitude, and time. On phase transformation under load and continuous hydrogen charging, local variations in the measured RA that can be associated with the loading mode and hydrogen concentration were observed. γ-Fe into α-Fe may be specifically localized near the crack tips requiring further studies.

MM 19.4 Tue 11:15 C 130

Hydrogen Effect on the Activation Enthalpy of Plastic Deformation — •Florian Schaefer, Rouven Schneider, Lukas Hasenfratz, and Christian Motz — Materials Science and Methods, Saarland University, Campus D2 3, 66123 Saarbruecken, Germany

The strain rate sensitivity of a material arises from a thermally activated contribution to the rate-determining deformation process, e.g. to dislocation slip or dislocation grain boundary interaction. For instance, nanocrystalline f.c.c. metals exhibit an increased strain rate sensitivity compared to a coarse-grained equivalent due to the constraints on dislocation plasticity caused by the multitude of grain boundaries. In this study, the extent to which hydrogen affects thermally activated dislocation mobility and thus the strain rate sensitivity was investigated. For this purpose, specimens were charged in situ, both cathodically and by low-pressure hydrogen plasma, and subjected to nanoindentation, micropillar compression, and strain-rate jump macro-tensile tests, and the results were contrasted. Hydrogen is shown to increase the strain rate sensitivity of f.c.c. nickel but not in a b.c.c structural steel. The temperature was then varied to the cryogenic level. For this purpose, the macro strain rate jump tests were carried out in a bath cryostat combined with ex situ charging. The low temperature prevents from outgassing. The activation volume for plastic deformation in a head-to-head comparison between nanocrystalline and coarsely grained f.c.c. nickel as well as the b.c.c. structural steel shows that the rate-determining deformation mechanism seems to change for f.c.c. but not for the b.c.c. material.

MM 20: Data Driven Material Science: Big Data and Workflows III

Time: Tuesday 10:15–13:00 Location: C 243

MM 20.1 Tue 10:15 C 243

Bulk and Surface Properties of cesium-telluride Photocathode Materials via High-Throughput Density Functional Theory Calculations — •Holger-Dietrich Sassnick[1] and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität Oldenburg, Physics Department, 26129 Oldenburg, Germany — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

Cesium-based photocathodes such as cesium-telluride are commonly used as electron sources in particle accelerators but the lack of knowledge of their crystal structure and stoichiometry during synthesis hinders their control. To predict which compounds are more likely to form and to characterize their properties, we apply a high-throughput workflow based on density functional theory calculations. Firstly, we calculate the formation energies and electronic properties of bulk phases obtained from computational databases employing the meta-GGA functional SCAN, which is known to provide accurate results for these systems [Saßnick & Cocchi, *Electron. Struct.* **3**, 027001 (2021)]. Our results indicate that a large number of different crystal structures may form and coexist in actual samples [Saßnick & Cocchi, *J. Chem. Phys.* **156**, 104108 (2022)]. In a second step, surface properties, which play a fundamental role in the photocathode performance, are calculated for a selected set of stable bulk crystals. The studied surfaces exhibit diverse properties ranging from semiconducting to metallic character with the latter being formed by facets terminated with an excess of metallic species.

MM 20.2 Tue 10:30 C 243

Thermodynamic and phonon properties of multi-alkali antimonides from density-functional theory and machine learning — •Julia Santana-Andreo, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics

Modern advancements in generating ultrabright electron beams have ushered in innovative experimental techniques in particle accelerators. However, the current challenge lies in improving the quality of electron sources primarily with novel photocathode materials, such as alkali-based semiconductors. In this work, we employ density functional theory combined with machine learning techniques to probe the thermodynamic stability of various alkali-based crystals, emphasizing the role of the approximations taken for the exchange-correlation (xc) functional. Our results reveal that SCAN offers the optimal trade-off between accuracy and computational costs to describe vibrational properties in these materials. Furthermore, it is observed that systems with a higher concentration of Cs atoms exhibit enhanced anharmonicities, which are accurately predicted and characterized with the employed methodology.

MM 20.3 Tue 10:45 C 243

Energetic and electronic properties of K-Sb and Na-Sb binary crystals from high-throughput ab initio calculations — •Richard Schier, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institut für Physik

The development of photocathode materials for the generation of ultrabright electron beams is essential for optimizing the performance of synchrotrons and thus to open unprecedented opportunities to access the fundamental properties of materials. Alkali-based photocathode materials have come into the limelight as novel semiconducting materials for electron sources. However, due to the complexity of the growth process, they are still poorly characterized. Ab initio methods can contribute to fill this gap offering a tool to simulate them without the need for empirical parameters. In this work, we investigate K-Sb and Na-Sb binary crystals taking as an input structures available from computational databases. Adopting a high throughput workflow based on density functional theory, we evaluate the energetic stability of the scrutinized materials discarding unstable structures. For the remaining ones, we analyze the electronic properties focusing on the correlation between band-gaps and material composition. By calculating the band structure and atom-projected density of states, we gain further insights into the electronic properties of these systems. Our results provide an insight into the numerous intermediate phases that can form when growing alkali-based photocathodes and allow us to better understand the growth process.

MM 20.4 Tue 11:00 C 243

Predicting Equilibrium Pressure for Hydrogen Storage: A Cheminformatics Approach Using Deep Neural Networks — •Sinan S. Faouri[1,2], Kai Sellschopp[2], Paul Jerabek[2], and Claudio Pistidda[2] — [1]Applied Science private University — [2]Helmholtz-Zentrum hereon

Hydrogen storage is a critical aspect of hydrogen-based energy systems, and predicting the equilibrium pressure during storage processes is essential for optimizing storage conditions. In this study, we employ a cheminformatics approach by extracting a comprehensive set of descriptors, including electronegativity, electron affinity, atomic radius, thermal conductivity, and more, to characterize the hydrogen storage process. These descriptors serve as inputs for deep neural networks (DNNs) to predict the equilibrium pressure. We compare the performance of the DNN model against three other machine learning models to assess its predictive capabilities. The evaluation metrics of all four models are thoroughly examined and compared, providing insights into their respective strengths and weaknesses. This comparative analysis aims to elucidate the effectiveness of the cheminformatics-driven DNN approach in predicting equilibrium pressure for hydrogen storage, contributing to the advancement of efficient and reliable hydrogen storage technologies. The findings of this study have broader implications for the development and optimization of hydrogen-based energy systems.

MM 20.5 Tue 11:15 C 243

Peeling back the layers; Incorporating Dispersion Interactions and Quantum Mechanics at Clay Mineral Interfaces. — •Sam Shepherd, Gareth. A Tribello, and David. M Wilkins — Queen's University Belfast, Belfast, Northern Ireland, BT7 1NN

Clay minerals are complex layered materials whose unique structures allow them to be used in a range of processes. Accurately describing the interactions which take place between their layers however, remains a challenge. When studying these minerals theoretically, the need for accurate dispersion interactions is well understood, but accounting for the necessarily large system sizes and long timescales has hitherto limited theoretical study into these minerals.

To rectify this, we created a family of machine learned interatomic potentials (MLIPs), trained using dispersion corrected DFT calculations. We used these potentials to minimise computational expense while studying kaolinite for extended timescales. Thus, we have obtained structural and dynamical properties of kaolinite with previously unachievable levels of accuracy. Due to the nature of the interlayer interactions, we performed path integral molecular dynamics (PIMD) to include nuclear quantum effects (NQEs). This allowed us to perform simulations of kaolinite while treating the system fully quantum-mechanically.

We find that the addition of NQEs significantly impacts the dynamical properties of the system. This finding conclusively shows the need for full quantum mechanical approaches to gain a better appreciation of mechanistic processes like adsorption.

15 min. break

MM 20.6 Tue 11:45 C 243

Experiment-driven atomistic materials modeling: Combining XPS and MLPs to infer the structure of a-CO$_x$ — •Tigany Zarrouk and Miguel Caro — Aalto University, Espoo, Finland

One facet of materials modelling is to gain insights from experimental results, which necessitates an effective strategy for identifying atomic structures that align with experimental data, *e.g.* spectra. Conventional approaches for amorphous materials involve generating numerous configurations through Molecular Dynamics and selecting one with the closest predicted spectrum to experiment. However, this process is inefficient and lacks assurance of spectrum conformity. We introduce a Grand-Canonical Monte Carlo methodology to generate configurations that concur with both experimental data and ab-initio calculations. Utilising a SOAP-based [1] X-Ray Photoelectron Spectroscopy (XPS) model trained on GW and Density Functional Theory (DFT) data, in conjunction with CO Gaussian Approximation Potential (GAP),

we identify oxygenated amorphous carbon structures compliant with experimental XPS predictions that are also energetically favourable within DFT. Clustering and embedding SOAP descriptors provides a data-driven deconvolution of the XPS spectrum into motif contributions, revealing the significant inaccuracies present in experimental XPS interpretation. This method generalises to multiple sets of experimental data and allows for the elucidation of specific experimental results, enhancing the applicability of materials modelling.
[1] Albert P. Bartók *et al.*: On representing chemical environments, Phys. Rev. B 87, 184115

MM 20.7 Tue 12:00 C 243

Exploring high-entropy alloy transport properties through the lens of machine learning — •Ruiwen Xie[1], Ye Wei[2], Bo Peng[3], Jiamu Liu[3], Liuliu Han[4], and Hongbin Zhang[1] — [1]Group of Theory of Magnetic Materials, Technical University of Darmstadt, Darmstadt, Germany — [2]École Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [3]State Key Laboratory of Tribology in Advanced Equipment, Tsinghua University, Beijing, China — [4]Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH

The high-entropy alloys (HEAs), or the compositionally complexed alloys (CCAs), have attracted much attention due to their multifunctional properties with a vast chemical space to explore. For instance, the five-component HEAs contain approximately 4.6 million compositional combinations with a 1 at.% interval. Therefore, efficient sampling methods to navigate the chemical space for optimized properties are needed. As a showcase, we establish a workflow by combining the multi-objective Bayesian optimisation (MOBO) and active learning (AL), in order to explore the Ta-Nb-Hf-Zr-Ti system for compositions with optimal spin Hall conductivities and spin Hall angles. Additionally, a Monte Carlo beam search based AL algorithm is used to explore FeCoNi-based HEAs targeting for high saturation magnetization, high anomalous Hall conductivity and low electrical conductivity simultaneously.

MM 20.8 Tue 12:15 C 243

Machine-learning structural stability of complex intermetallic phases — •Mariano Forti, Ralf Drautz, and Thomas Hammerschmidt — ICAMS, Ruhr-Universität Bochum. Universitätsstr. 150 44801 Bochum

The understanding of the precipitation of topologically close packed (TCP) phases in single-crystal superalloys is of central importance for the design of these materials for high-temperature applications. However, the structural complexity of these intermetallic compounds and the chemical complexity of the superalloys with typically up to ten elements hampers the exhaustive sampling of chemical space by density-functional theory (DFT) calculations. For example, the computation of the convex hull of the R phase with 11 inequivalent lattice sites would require N^{11} DFT calculations in an N-component system. We overcome this computational limitation by combining machine learning (ML) techniques with descriptors of the local atomic environment of the TCP phases. In particlar, we use descriptors derived from bond order potentials (BOP) and atomic cluster expansions (ACE) that retain structural and electronic information. The resulting ML models predict the relative stability of complex TCP phases with very good precision in binary and ternary systems even for small training-data sets of only few hundred data points. We explore strategies for knowledge based feature selection that make it possible to handle the exponentially growing number of features in multicomponent systems, and to obtain a prediction for the convex hull of the R phase in Cr-Co-W system.

MM 20.9 Tue 12:30 C 243

Influence of the neighboring phases of MnS inclusions on damage accumulation in case-hardening steel — •Clara Reinhart[1], Tom Reclik[1], Maximilian A. Wollenweber[1], Ulrich Kerzel[2], Talal Al-Samman[1], and Sandra Korte-Kerzel[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Aachen, Germany — [2]Data Science and Artificial Intelligence in Materials and Geoscience, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Aachen, Germany

Microstructural damage sites that are created during forming processes are usually observable in the form of voids and known to impede the mechanical properties of materials, especially during cyclic and rapid loading. In the case of 16MnCrS5 case-hardening steel, MnS inclusions lead to the creation of damage sites by cracking or delamination due to a pronounced mechanical contrast in the microstructure. This mechanical contrast depends on whether the inclusion is surrounded by ferrite, pearlite or both phases simultaneously. In this work we set out to characterize damage sites based on the neighboring phase of the MnS inclusion by training a machine learning network to automatically segment the etched microstructure and characterize the interfaces. In a second step damages sites are automatically detected and correlated to the determined neighboring phase(s). With this approach we show that a large difference of damage accumulation emerges for different neighboring phases, distinguishing not only inclusions with one-phase and two-phase interfaces, but also inclusions surrounded exclusively by either ferrite or pearlite.

MM 20.10 Tue 12:45 C 243

High-throughput damage quantification in steel and opportunities for damage-controlled forming processes — •Maximilian A. Wollenweber[1], Jannik Gerlach[2], Tom Reclik[1], Clara Reinhart[1], Sebastian Münstermann[2], Talal Al-Samman[1], and Sandra Korte-Kerzel[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Aachen, Germany — [2]Institute of Metal Forming, RWTH Aachen University, Aachen, Germany

When trying to improve the mechanical properties of steel parts a frequently overlooked cause for degradation of mechanical properties is the prevalence of damage sites often present in the form of voids in the microstructure. Caused by the mechanical contrast of different phases leading to plastic inhomogeneities during the forming process, these damage sites majorly decrease the longevity and crash performance. Trying to reduce these damage sites to enable damage-controlled forming processes poses two big challenges: On the one hand damage sites need to be characterized in order to understand the microstructural effects on damage formation and growth. On the other hand, optimized strain paths and adjusted microstructures need to be conceptualized to minimize the effect of damage on the performance. In this work we want to exemplary show how to tackle both of these issues; how high-throughput scanning electron microscopy and artificial intelligence can be used to evaluate damage sites, as well as demonstrating how adjustments to the strain-path and different microstructural concepts harbor opportunities for damage-controlled forming processes.

MM 21: Transport in Materials: Diffusion, Conduction of Charge or Heat I

Time: Tuesday 10:15–11:30 Location: C 264

MM 21.1 Tue 10:15 C 264

Transport and diffusion in the two-dimensional Hubbard model — •Martin Ulaga[1], Jernej Mravlje[1,2], Peter Prelovšek[1], and Jure Kokalj[3,1] — [1]Insitute "Jožef Stefan", Ljubljana, Slovenija — [2]Faculty of mathematics of physics, University of Ljubljana, Ljubljana, Slovenija — [3]Faculty of civil and geotedic engineering, University of Ljubljana, Ljubljana, Slovenija

We study transport coefficients and diffusion constants in the square lattice Hubbard model by using the finite-temperature Lanczos method and Nernst-Einstein relations. Notably, we observe a strong, non-monotonic temperature dependence in heat conductivity that violates the Mott-Ioffe-Regel limit across a wide range of parameter space, mirroring the behavior of charge conductivity. These findings are particularly significant for experiments on cold-atomic gases, as well as on cuprates. We comment on the experimental implications of our results for thermal conductivity in the Mott-insulating regime and the Lorenz ratio in the doped Mott insulator.

MM 21.2 Tue 10:30 C 264

Transport mechanism in Lithium thiophosphate — •Davide Tisi, Lorenzo Gigli, Federico Grasselli, and Michele Ceriotti — Ecole Polytechnique Federale de Lausanne (EPFL)

Lithium ortho-thiophosphate (Li3PS4) are a promising candidate for solid-state-electrolyte batteries. The microscopic mechanisms of Li-ion transport in Li3PS4 are, still, far from being fully understood, and no computational work has tackled the thermal conductivity at DFT level.

In this talk, I will show how we build multi-level machine learning potentials targeting state-of-the-art DFT references (PBEsol, SCAN, and PBE0), to study the electrical and thermal conductivity of all the known phases of Li3PS4 (α, β and γ). I will discuss the physical origin of the superionic behaviour of Li3PS4: the activation of PS4 flipping drives a structural phase transition to a highly conductive phase, characterised by an enhancement of Li-site availability and by a drastic reduction in the activation energy of Li-ion diffusion. I will show the effects of the phase transition on both the electrical and thermal conductivity. We elucidate the role of inter-ionic dynamical correlations in charge transport, by highlighting the failure of the Nernst-Einstein approximation to estimate the electrical conductivity. Finally, we compare the thermal conductivity computed by the Green-Kubo theory with the results from the Boltzmann transport equation, to highlight the role of anharmonicity and quantum effects.

Our results show a dependence on the target DFT reference, with PBE0 yielding the best quantitative agreement with experiments.

MM 21.3 Tue 10:45 C 264

Phonon anharmonicity at lower mantle conditons: Consequences on the thermal conductivity of MgO — •Saadi Chabane, Paola Giura, Lorenzo Paulatto, and Daniele Antonangeli — Institut de minéralogie, de physique des matériaux et de cosmochimie, Sorbonne université, Paris, France

Understanding the properties of Magnesium oxide's (MgO) properties is essential for planetary sciences and technology, especially as a fundamental component in Earth's lower mantle (LM). This discussion explores the complex field of anharmonic effects due to phonon scatterings in MgO, specifically addressing their behavior under extreme high-pressure and high-temperature LM conditions. The objective is to determine the influence of these anharmonicities on lattice thermal conductivity. Conducting ab-initio analyses for two distinct scenarios: one simulating elevated temperatures up to 1223K and another replicating LM conditions with T-P values ranging from 1900K-24GPa to 3000K-130GPa. Our study employs Infrared and inelastic x-ray scattering observations performed in our team for benchmarking. A comparison with simulations validates joint Density Functional Perturbation Theory (DFPT) and self-consistent harmonic approximation (SSCHA) computations for vibrational energies and phonon lifetimes, ensuring theoretical predictions align with experimental data. Additionally, a simplified model is utilized to explore the impact of mass disorder on thermal conductivity. Descending into the lower mantle, our findings unveil an unexpected change in anharmonic properties, attributed to the interplay of extreme pressure and temperature.

MM 21.4 Tue 11:00 C 264

Strong Quartic Anharmonicity and Thermoelectric Performance in Antiperovskite — •Wenling Ren[1], Jincheng Yue[2], Shuyao Lin[1,3,4], Chen Shen[1], Yanhui Liu[2], Tian Cui[2], Harish Kumar Singh[1], Terumasa Tadano[5], and Hongbin Zhang[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Ningbo University, Ningbo, China — [3]TU Wien, Vienna, Austria — [4]Linkoping University, Linkoping, Sweden — [5]National Institute for Materials and Science, Tsukuba, Japan

Antiperovskite(APV) materials have garnered significant attention due to their rich physical properties. We employed a combination of SCP theory and the BTE, ultimately evaluating the thermal and electronic transport properties of APV (A_3XN,A=Mg,Ca,Sr;X=P,As,Sb,Bi). It is observed that such materials stand out for their strong quartic anharmonicity, stemming from the underlying exceptional lattice distortion. This leads to a relatively subdued temperature response concerning the lattice thermal conductivity, especially at elevated temperatures. Detailed analysis is done by investigating the dynamical stability and phonon scattering properties to elucidate the origin of reduced thermal conductivities. Further calculations on the electronic transport properties reveal that such materials exhibit promising thermoelectric figure of merit, i.e., up to 1.25, 1.03 and 1.03 for Ca_3BiN, Mg_3BiN and Sr_3BiN, respectively. Our work serves as a proof-of-concept example of a comprehensive exploration of APV materials, suggesting their significant potential for future medium/high-temperature thermoelectric applications.

MM 21.5 Tue 11:15 C 264

Role of anharmonicity in the lattice dynamics and thermal transport of different phases of $KNbO_3$ — •Niloofar Hadaeghi, Chen Shen, and Hongbin Zhang — Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

The $KNbO_3$ material, with its intriguing properties, has always been considered as a great (lead-free) candidate in the energy storage applications. However, despite the significant interest in its cubic, tetragonal, and orthorhombic phases, investigation of their lattice dynamics and lattice thermal transport have remained challenging, due the unstable phonon modes in the harmonic phonon dispersion bands. Here, utilizing self-consistent phonon theory and compressive sensing techniques, we explore the significant role of quartic anharmonicity in the renormalization of the harmonic interatomic force constants and hardening of the lattice modes in the temperature dependent phonon bands and density of states in the three phases. Moreover, the lattice thermal conductivity (LTC), along with the phonon lifetimes are studied for the three phases. The achieved results are in a good agreement with experimental values, where the lower experimental values are due to the higher different types of scattering related to the poly-crystalline nature in the experiment. For instance, the calculated result at 1000 K is 1.45 W/m.K for the cubic phase, where the experimental value is 1.2 W/m.K. The values of LTC at 300 K are as 4.2 W/m.K for the cubic, 7.3 W/m.K for the tetragonal and 7.8 W/m.K for the orthorhombic phases.

MM 22: Interface Controlled Properties, Nanomaterials and Microstructure Design III

Time: Tuesday 10:15–11:30 Location: C 230

MM 22.1 Tue 10:15 C 230

Strain engineering for CMOS microelectronics — •Costanza Manganelli[1], Ignatii Zaitsev[1], Agnieszka Anna Corley-Wiciak[1], Cedric Corley-Wiciak[2], Marvin Hartwig Zoellner[1], Carsten Richter[3], Edoardo Zatterin[2], Michele Virgilio[4], Beatriz Martin-Garcia[5], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [2]ESRF -European Synchrotron Radiation Facility, Grenoble, France — [3]IKZ -Leibniz -Institut für Kristallzüchtung, Berlin, Germany — [4]Università di Pisa, Pisa, Italy — [5]CIC nanoGUNE BRTA & IKERBASQUE, Basque Country, Spain

The significance of strain engineering in CMOS microelectronics extends across diverse applications, encompassing opto-electronics, sensing, and quantum technologies, and a variety of materials from SiGeSn semiconductors to 2D materials (MoS2, hBN and perovskites). Experimental analyses (Photoluminescence, Raman, X-Ray Spectroscopy) and simulation platforms enable the prediction and optimization of material processes and device design. We present a systematic study elucidating how the temperature-dependent distribution of strain can impact the optical and transport performance of semiconductor devices. Our investigation focuses on strained Ge microdisks, crucial components for developing guidelines for integrated light emitters. We also explore the role of metal electrodes in quantum confinement buses within CMOS-compatible devices. This research provides valuable insights into strain effects on semiconductor devices, laying a foundation for developing and optimizing future microelectronic devices.

MM 22.2 Tue 10:30 C 230

A theoretical analysis on the bulk photovoltaic effect in strained microstructures — •Ignatii Zaitsev[1], Davide Spirito[1], Jacopo Frigerio[2], Carlos Alvarado Chavarin[1], Michele Virgilio[3], Anke Lüdge[4], Wolfgang Lüdge[4], Raffaele Giani[2], and Costanza Lucia Manganelli[1] — [1]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [2]L-NESS, Dipartimento di Fisica del Politecnico di Milano, Polo Di Como, Italy — [3]Università di Pisa, Pisa, Italy — [4]LPCon GmbH, Berlin, Germany

Strain engineering in microstructures is a powerful tool for optimization of electronic and optical properties in semiconductor devices. We propose a proof of concept for the development of a cost-effective, compact, fast, and non-destructive approach to probe non-uniform strain fields in semiconductors, exploiting the bulk photovoltage effect. We show a benchmark case represented by an array of silicon nitride stripes deposited at different pressure conditions on a germanium substrate. First, we verify their surface deformations by means of Raman spectroscopy; secondly, we reproduce that in a finite element method simulation platform by combining mechanical simulations with deformation potential theory to then estimate the band edge energy landscape. Finally, we discuss theoretical behavior of the photovoltage signal based on the semiconductor sample characteristics such as defects and doping as well as deformation.

MM 22.3 Tue 10:45 C 230

Influence of Trench Geometry on the Directed Capillary Self-Assembly of Anisotropic Gold Nanoparticles — •Stefan M. Schupp[1], Felizitas Kirner[2], Helmut Cölfen[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, Germany

The self-assembly of anisotropic metal nanoparticles (NPs) into ordered nanostructures is a promising bottom-up approach for applications in photonics and nanoelectronics due to the unique directional properties of the resulting structures. However, the deterministic placement and orientation of these NPs remains a challenge to this day. In this study, we apply a combination of capillary forces and lithographically patterned substrates to assemble gold nanocubes (AuNCs) with an edge length of 60 nm into linear structures. Here, the influence of trench geometry on the assembly outcome is investigated in detail, which allows to generate ordered mono- to bilayer AuNC structures with varying widths. Finally, this directed capillary self-assembly approach is used to assemble AuNC lines onto pre-fabricated electrodes to perform electrical measurements. Thus, this method can be applied to integrate anisotropic NPs into future electronic devices.

MM 22.4 Tue 11:00 C 230

Electronic properties of transition metal dichalcogenide nanowrinkles — •Stefan Velja[1], Jannis Krumland[2], and Caterina Cocchi[1,2] — [1]Institute of Physics, Carl von Ossietzky Universität Oldenburg — [2]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin

Mechanical deformations in transition metal dichalcogenide monolayers can appear both spontaneously and artificially, giving rise to structures such as nanowrinkles or nanobubbles. Such deformations have been observed to harbor localized electron states, a known prerequisite for single-photon emission, triggering theoretical studies attempting to explain these phenomena. However, fully quantum-mechanical insight given by ab initio calculations is still missing to date.

We model one-dimensional MoSe2 nanowrinkles by applying uniaxial compressive strain with increasing magnitude in the plane of the monolayer. We analyze their structural properties highlighting the effects of coexisting local domains of tensile and compressive strain in the same system. We find that the electronic properties are driven by the curvature rather than strain: band gaps vary moderately in size compared to flat counterparts and remain direct: in contrast, the spatial distribution of the frontier states is affected by strain. We finally discuss transport properties through the inspection of effective masses and their correlation with wave-function distributions, showing the excellent perspectives for these systems as active components for (opto)electronic devices.

MM 22.5 Tue 11:15 C 230

Electric field gradients at ^{111m}Cd sites in single domain and periodically poled Mg-doped LiNbO$_3$ crystals — •Hannes Gürlich[1], Björn Dörschel[3], Thienh Thanh Dang[3], Ian Yap[3], Juliana Schell[1,2], Samuel Dominic Seddon[1], Boris Koppitz[1], and Lukas Eng[1] — [1]Technische Universität Dresden — [2]European Organization for Nuclear Research (CERN) — [3]Instrute for Materials Science and Center tor Nanointegration Duisburg-Essen (CENIDE)

At ISOLDE-CERN, ^{111m}Cd was implanted at 30 keV into differently ferroelectric-polarized LiNbO$_3$-5%Mg crystals in z-direction. After annealing at 600 °C, 700 °C or 800 °C for up to 30 min in an oxygen atmosphere, the samples were measured with the time-differential perturbed angular correlation (TDPAC) technique for at least 2 h at room temperature.

The results show that in the periodically polled samples, the measured electric field gradient (EFG) is strongly suppressed. While in the single domain samples, this depends strongly on the annealing temperature. At 800 °C annealing temperature, the signal is strongly suppressed, while at 700 °C the best results were found. Therefore, it is proposed, that in between those two temperatures an irreversible destruction of the unitary directed polarization occurs.

Two main frequencies were found being independent of the polarization direction: 214(5) MHz and 173(5) MHz.

MM 23: Topical Session: Hydrogen in Materials: from Storage to Embrittlement III

Time: Tuesday 11:45–13:15 Location: C 130

Topical Talk MM 23.1 Tue 11:45 C 130

Hydrogen trapping evaluation by thermal desorption spectroscopy coupled with advanced microstructural characterization: from BCC to FCC — Liese Vandewalle, Margot Pinson, Simon Vander Vennet, Lisa Claeys, Kim Verbeken, and •Tom Depover — Technologiepark 46, 9052 Zwijnaarde, Ghent University, Belgium

The most used technique to evaluate hydrogen trapping is thermal desorption spectroscopy (TDS). However, based on the TDS spectrum itself, one can find a variety of possible hydrogen trapping sites linked to specific microstructural features. Therefore, TDS should always be combined with advanced microstructural characterization to elucidate the hydrogen/metal interactions, where variations in defect density should be coupled with a corresponding increase/decrease in the TDS profile. In this work, the hydrogen trapping ability of a wide range of metals is considered, starting from ultra-low carbon steel (pure ferrite, BCC), over high carbon martensitic steels (BCT), towards the role retained austenite (FCC) can play in advanced high strength Q&P steels, ending with limitations of the technique in a pure austenitic microstructure. This is coupled with the characterization of the microstructure, studied by combined internal friction, positron annihilation spectroscopy, SEM-EBSD, XRD, DSC and TEM.

MM 23.2 Tue 12:15 C 130

Hydrogen sorption kinetics in nanoporous palladium — •Seoyun Sohn[1], Jürgen Markmann[1,2], Shan Shi[3,1], and Jörg Weissmüller[2,1] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany

Palladium is one of the most intensely studied model materials for hydrogen in metals. The fabrication of nanoporous Pd by dealloying results in a macroscopic sample with a nanoscale network structure, which can efficiently absorb hydrogen due to its large specific surface area and short diffusion paths. The material has been reported to undergo more than 1000 loading/unloading cycles through the α/α' phase transformation without degradation. In this work, the ligament size of nanoporous Pd is tuned from 20 to 500 nm with the aim of understanding the role of the geometry on the charging kinetics and ultimately on the phase transformation mechanism. The hydrogen ad/absorption and desorption kinetics are studied using electrochemical impedance spectroscopy and potential jump tests. The results suggest a controlling role of the interfacial injection process and an extremely small Damköhler number. This outcome will offer guidance to improve charging kinetics for functional performance.

MM 23.3 Tue 12:30 C 130

Influence of Varying Conditions on Kinetics of Reactive Hydride Composites — •Ou Jin[1,3], Yuanyuan Shang[2], Xiaohui Huang[3], Dorothée Vinga Szabó[1,3,4], Thi Thu Le[2], Stefan Wagner[1], Christian Kübel[3,4,5], Claudio Pistidda[2], and Astrid Pundt[1,3] — [1]Institute for Applied Materials, KIT — [2]Institute of Hydrogen Technology, hereon — [3]Institute of Nanotechnology, KIT — [4]Karlsruhe Nano Micro Facility, KIT — [5]Joint Research Laboratory Nanomaterials, TUD

A sustainable energy future necessitates the incorporation of hydrogen as a critical energy vector. However, its widespread use is restricted by available storage techniques. The LiBH4-MgH2 composite, among the reactive hydride composites, possesses an exceptional storage capacity of about 12 wt% H2 while using milder operating conditions compared to current commercial solutions. However, the material's practical application is hindered by sluggish kinetics due to the slow formation of MgB2 during dehydrogenation. Facilitation of MgB2 formation was proposed through transition metal-based additives to expedite the LiBH4-MgH2 dehydrogenation. Despite of this, the mechanism underpinning these improvements was not fully explored at the time. This research investigates the effect of variables such as the kind of additive, annealing temperature, and cycling on the MgB2 formation during the decomposition of LiBH4-MgH2 using various transmission electron microscopy (TEM) techniques. The analysis reveals that the improved kinetics in the material results from the tuned nucleation and growth behavior of MgB2, due to different MgB2 nucleation behaviors.

MM 23.4 Tue 12:45 C 130

The role of manganese and aluminium on hydrogen trapping and diffusion in Mn/Al rich steel alloys — Bikram Kumar Das[1], •Mauricio Bonilla[1], Poulami Chakraborty[1], and Elena Akhmatskaya[1,2] — [1]BCAM - Basque Center for Applied Mathematics, Bilbao, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Hydrogen-induced embrittlement (HIE) remains a serious bottleneck for using steel in infrastructure for H_2 storage and transport. Small amounts of Al and Mn have been shown to mitigate HIE, but the proposed mechanisms are often contradictory. To address this problem, we present a systematic approach to model the local environments (LEs) around the H-binding sites in FCC Fe-Mn-Al alloys up to the 3^{rd} nearest neighbor (NN) shell. First, the most favorable LEs are determined using Density Functional Theory (DFT). Then, the local impact of Al/Mn content and distribution on the binding and diffusion of H is examined through the nudge elastic band method and crystal orbital Hamilton population analysis. We found that H-binding correlates most strongly with Al content, and is weakly influenced by Mn up to 5 wt%. Moreover, direct H-Al bonding destabilizes H binding, but the presence of Al in the 2^{nd} NN shell of the H-binding site leads to a strong stabilizing effect by promoting H-Fe bonding. The presence of Al and Mn in grain boundaries and precipitates is known to play a prominent role in HIE. Here, we show that Al ability to indirectly trap H in bulk austenite could mitigate HIE. The analysis approach in this work could readily be adapted to study similar alloy systems.

MM 23.5 Tue 13:00 C 130

Unprecedented switchable rigidity in a nanoporous Pd alloy-hydrogen solid solution near critical point — •Sambit Bapari[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

A remarkable prediction due to Larché and Cahn is deformation at no cost of energy at the critical point for open systems with miscibility gaps. Bulk nanoporous palladium is an ideal system for studying open system elasticity as palladium with randomly oriented nanometer size ligaments affords rapid equilibration of hydrogen between an environment and the materials bulk. In this work, nanoporous Pd-Pt (5 at%) alloy with residual Cu (13 at%) was prepared by electrochemical dealloying to experimentally verify the prediction for a wide solute-concentration range. The average ligament size of the as dealloyed nanoporous alloy is ˜ 4 nm, facilitating fast equilibration with the acidic electrolyte present in the open pores under applied potential. Hydrogen solubility isotherms show near critical point behavior in the Pd-Cu-Pt-H solid solution at room temperature. Solute susceptibility and concentration-strain coefficient were determined to estimate the difference in stiffness between open and closed systems. In-situ dynamic mechanical tests show an unprecedented 50% drop in the storage modulus owing to simultaneous mechanical and chemical equilibration near critical point.

MM 24: Transport in Materials: Diffusion, Conduction of Charge or Heat II

Time: Tuesday 11:45–13:15 Location: C 264

MM 24.1 Tue 11:45 C 264

Towards Highly Conductive Graphite Films: Tungsten Carbide Doping of Thermally Reduced Graphene Oxide Paper — •Leonhard Niemann[1,2], Tianshan Xu[1,3], Markus Gruschwitz[2], Martin Köhne[1], and Christoph Tegenkamp[2] — [1]Robert Bosch GmbH, Department of Advanced Technologies and Micro Systems, 71272 Renningen — [2]Technical University of Chemnitz, Institute of Physics, 09107 Chemnitz — [3]RWTH Aachen, Gemeinschaftslabor für Elektronenmikroskopie GFE, 52062 Aachen

The growth of consumer electronics and the electrification of transport has increased enormously the demand for copper. This will lead to a global shortage of this element. Graphene-based conductors are an interesting lightweight and low-cost alternative. However, the electrical conductivity values achieved to date are not sufficient to compete with traditional copper-based conductors. To increase the electrical conductivity, various additives are under research. This study delves into the synergistic effects of tungsten carbide (WC) doping on the graphitization process of graphene oxide (GO) films. Tungsten, a well-known catalyst for promoting graphitization in amorphous carbon structures, holds promise for advancing the properties of graphene-based materials. We focused on optimizing the concentration of W to facilitate the graphitization of GO films. The samples were subjected to controlled thermal treatments, and their structural evolution was characterized. The resulting WC/graphite films with a conductivity of 432 to 594 kS/m demonstrate a concentration-dependent effect, with an optimal concentration range of 1 to 3 μmol/mg of WS$_2$ in GO.

MM 24.2 Tue 12:00 C 264

Charge transport simulation using kinetic Monte Carlo with fast update rules — •Roya Ebrahimi Viand, Karsten Reuter, and Sebastian Matera — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The diffusion of particles in a solid material is often characterized by rare jumps between low-energy sites, which allows for the simulation of long-time dynamics using the kinetic Monte Carlo (kMC) methodology. In the case of charged particles, kMC can become costly because the long-range Coulomb interaction requires recalculating all process rates in every kMC step, despite the fact that each step introduces only local changes in the system's state. In this talk, we introduce update rules for, in general, anisotropic lattices, which require only two element-wise vector multiplications. This can be implemented very efficiently on modern compute architectures, and we discuss this using a newly developed kMC framework. We demonstrate the approach on a first-principles kMC model for Li$^+$ transport in graphite in a high state of charge and investigate the dependence of mobility on the charge carrier density.

MM 24.3 Tue 12:15 C 264

Chiral anomaly induced monopole current and nonlinear circular dichroism — •Nikolai Peshcherenko[1], Claudia Felser[1], and Yang Zhang[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]University of Tennessee, Knoxville, Tennessee 37996, USA

Topological Weyl and Dirac semimetals are known to demonstrate a chiral anomaly effect subject to parallel electric and magnetic fields. The most well-known experimental probe of this effect is large negative longitudinal magnetoresistance. However, due to other strongly nonisotropic contributions to magnetoresistance existing in semimetals it could be interesting to consider other possible types of chiral anomaly experimental manifestations.

We suggest a simple chirality probe in TR invariant Weyl and Dirac semimetals with nonlinear Hall response. We demonstrate that chiral anomaly-induced relative shift of Weyl cones in energy space gives rise to chirality-asymmetric intranode momentum relaxation times. Due to this asymmetry, proportional to anomalous velocity Hall currents excited by external electric fields in different Weyl nodes do not perfectly compensate each other. We predict that this effect could be also observed in circular dichroism measurements.

MM 24.4 Tue 12:30 C 264

spin Hall effect in antiferromagnetic alloys — •Nabil Menai[1], Martin Gradhand[1], and Derek Stewart[2] — [1]University of Bristol, Bristol, UK — [2]Western Digital Research Center, San Jose, CA, USA

Historically, antiferromagnets (AFM) were believed not to exhibit any anomalous Hall conductivity (AHC). Conversely, ferromagnets have been known for a long time to show a transverse voltage without the need for a magnetic field. Very recently, however, it was shown that some AFMs can indeed manifest AHC. Furthermore, AFMs could serve as a promising component for next-generation spintronics devices, thanks to their scalability, robustness against external magnetic fields, and ultrafast spin dynamics.

In this work, we employ density functional theory and Green function methods to calculate the transport properties of Mn based binary alloyed AFMs, specifically focusing on the spin Hall conductivity (SHC). Our goal is to identify a suitable AFM for spintronic applications that exhibits a high spin Hall angle (SHA).

Our findings indicate that doping MnPt with Pd can increase the SHA from around 2% to 5%. This enhancement should be experimentally observable, particularly at room temperature where the effect is further amplified, resulting in the SHA reaching around 8%. Additionally, we present examples of AFM materials in which non-symmorphic symmetries give rise to topological features such as the emergence of Dirac nodal lines, or even a new magnetic phase termed altermagnetism. These nodal lines have been shown to substantially enhance the SHC, offering potential applications in the field of spintronics.

MM 24.5 Tue 12:45 C 264

Exploring the tunability of the electronic properties of ZrSiSe — •Davide Pizzirani[1,2], Oleksandr Zheliuk[1,2], Julia Kreminska[3], Pim van den Berg[1,2], Claudius Müller[1,2], Maarten van Delft[1,2], Ratnadwip Shinga[4], Yu-Te Hsu[1,2], Leslie Schoop[4], Justin Ye[3], Nigel Hussey[1,2,5], and Steffen Wiedmann[1,2] — [1]HFML-FELIX, Radboud University, 6525 ED Nijmegen, the Netherlands. — [2]Institute for Molecules and Materials, Radboud University, Nijmegen 6525AJ, the Netherlands. — [3]Device Physics of Complex Materials, Zernike Institute for Advanced Materials, Nijenborgh 4, 9747 AG, Groningen, the Netherlands. — [4]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA. — [5]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom.

The interplay of topology and electronic correlations, as well as the transport properties of charge carriers with a linear dispersion, can be unraveled in nodal line semi-metals, such as ZrSiSe. We present thickness- and gate-dependent magneto-transport experiments up to 35 T on exfoliated high-quality thin flakes of ZrSiSe, with sample thicknesses ranging from 112 to 27 nm. In order to further investigate the tunability of the charge carrier properties in ZrSiSe, we additionally employ the ionic-liquid gating technique. As a function of thickness and applied gate voltage, we observe strong deviation from the quadratic magneto-resistance expected for compensated semimetals as well as an alteration of the Fermi surface, evidenced by a shift in the quantum oscillation spectra.

MM 24.6 Tue 13:00 C 264

Violation of Boltzmann quasi-particle transport in disordered alloy — •Gabor Csire[1], Franco Moitzi[1], Andrei Ruban[1,2], and Oleg Peil[1] — [1]Materials Center Leoben Forschung GmbH, Roseggerstraße 12, 8700 Leoben, Austria — [2]KTH Royal Institute of Technology, Brinellvagen 23, SE-100 44 Stockholm, Sweden

High resistivity disordered metals often exhibit deviations from the transport behavior described by the semiclassical Boltzmann theory. Here the scattering events from impurities or phonons cannot be treated as independent processes as suggested by Matthiessen's rule. The most extreme example of such a behavior are crystalline metallic alloys that exhibit a crossover from the positive to negative sign of the temperature coefficient of resistivity that persists from low to high temperatures. Various mechanisms, including weak localization and polaronic effects, have been put forward to explain the behavior within the framework of the Boltzmann transport theory but since most of these studies were relying on simple models a clear physical picture and quantitative material-specific description are still missing. In this contribution, we investigate the temperature-dependent resistivity of such „anomalous" alloys using our recent implementation of the Kubo-Greenwood formalism within the Korringa-Kohn-Rostoker method using Andersen's muffin-tin-orbital representation. In particular, we examine the temperature evolution of the non-Boltzmann transport contributions and discuss the origin of the sign change in the temperature coefficient.

MM 25: Interface Controlled Properties, Nanomaterials and Microstructure Design IV

Time: Tuesday 11:45–13:00 Location: C 230

MM 25.1 Tue 11:45 C 230

Automatic exploration of elementary processes with adaptive kinetic Monte Carlo — •King Chun Lai, Sebastian Matera, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Lattice kinetic Monte Carlo (kMC) is very efficient for the simulation of rare event controlled dynamics but requires prior knowledge about the network of elementary processes. Currently, constructing such a network heavily relies on human intuition, which has its limitations in complex scenarios. We address this with a newly developed adaptive kMC (akMC) framework to automatically explore the reaction space. Elementary processes are identified solely on the basis of their energetics and without human bias. A key feature of our akMC framework is the on-the-fly labeling of local atomic environments, which is used to speed up the process searching algorithm. Demonstrating on island migration on Pd surfaces, we employ this labeling to structure the obtained elementary processes. Intriguingly, the process exploration readily identifies a number of non-trivial elementary steps, which involve collective motion of multiple atoms in a single event. Long time scale kMC simulations including these collective processes highlight the shortcomings of prevalent human-generated fixed process lists which typically center on intuitive single-atom events.

MM 25.2 Tue 12:00 C 230

Rapid Metal-Induced Crystallization and Layer Exchange via Flash Lamp Annealing — •Max Stöber[1], Matthias Zschornak[2], Hartmut Stöcker[1], Felix Bräuer[1], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg — [2]Technische Physik, Hochschule für Technik und Wirtschaft Dresden, Friedrich-List-Platz 1, 01069 Dresden

DC sputtered Si layers are crystallized in the presence of a thin aluminum layer on a copper foil substrate. The energy for the reaction was provided by the means of Flash Lamp Annealing (FLA) technique with a pulse duration of 1 ms. X-Ray diffraction and scanning electron microscopy revealed structural changes, namely metal-induced crystallization and layer exchange. Above a certain flash energy the formation of a metastable intermetallic alloy was observed. The final synthesis result is an intermetallic alloy layer in between two metal layers, which can be refered to as a self-assembled sandwich structure. The metastable phase is "frozen in" due to rapid quenching. Some properties of the intermetallic layer can be fine-tuned by the flash lamp parameters. Understanding the fundamental processes involved may lead to interesting applications in heterostructured functional material systems.

MM 25.3 Tue 12:15 C 230

Nano-scale investigation of fractal abnormal grains and grain boundaries in Pd-Au using atom probe tomography — •Johannes Wild[1], Torben Boll[1,2,3], Fabian Andorfer[4], Svetlana Korneychuk[2,3], Jules M. Dake[4], Dorothée Vinga Szabo[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and Astrid Pundt[1,2] — [1]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, Ulm University

Nanocrystalline (NC) Pd-Au prepared by inert gas condensation exhibits fractal abnormal grain growth during heat treatment. The resulting microstructure is characterized by a bimodal grain size distribution with micrometer-sized grains (FG) embedded in a matrix of NC grains (NG). To elucidate this unusual manifestation of grain growth, we extracted sharp tip samples from FG and NG bulk regions, as well as from the FG-FG and FG-NG interface regions and analysed them with a LEAP 4000X HR atom probe. The NG region exhibited an O content that was multiple times higher in comparison with the FG region. Cluster analysis confirmed the presence of a multitude of O-rich clusters in the NG, but not in the FG region. Furthermore, the reconstructions of the boundary regions revealed an unexpected diversity of host and contamination element distributions at the FG-FG and FG-NG interfaces.

MM 25.4 Tue 12:30 C 230

Positive and Negative Structured 3D Nano Current Collectors Based on AAO Templates Applied for Sodium Metal Anodes — •Mo Sha and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The uncontrollable dendrite growth leads to safety issues during plating/stripping processes, severely restricting the practical application of sodium metal batteries (SMBs). 3D nano current collectors exhibit great potential for stabilizing the Na anode by homogenizing the electric field and Na ion flux distribution. Herein, 3D nanopore arrays (NPAs) and 3D nanorod arrays (NRAs) current collectors with opposite structures have been prepared with the AAO-template-assisted method. As current collectors for SMBs, both 3D NPAs and 3D NRAs have better electrochemical performance than 2D foil, demonstrating the great potential of 3D nanostructured current collectors based on AAO templates for SMBs. Compared with 3D NRAs, 3D NPAs have better electrochemical performance at a certain depth, with a long cycling stability of 1000 cycles at 1 mAh*cm-2 and 1 mA*cm-2 and a small nucleation potential of about 2 mV.

MM 25.5 Tue 12:45 C 230

effect of crack-tip geometry on crack-interface interactions in molecular dynamics studies of fracture in Ti-Al alloys — •Onur Can Şen[1,2] and Rebecca Janisch[2] — [1]IMPRS SusMet, Max-Planck-Institut für Eisenforschung GmbH — [2]ICAMS, Ruhr-Universität Bochum

The fracture behavior of lamellar Ti-Al alloys is strongly influenced by the twin interfaces in the microstructure. Molecular dynamics (MD) simulations are a valuable tool to systematically study crack-interface interactions with atomistic resolution, but their results are often criticized as being too academic. Experimental validation is difficult, because controlling the initial notch orientation is very challenging and the crack tip is never as sharp as in the typical MD set-ups. We investigate this issue by studying crack-tip interface interactions at various coherent and semi-coherent interface types in nano-lamellar Ti-Al, using different crack configurations to differentiate the effects of the microstructure from those of the crack geometry. Results show that the semi-coherent pseudo twin (PT) interface is the strongest barrier for crack propagation while the coherent true twin (TT) interface is the weakest. The initial crack orientation has a bigger influence on this effect than the aspect ratio of the microcrack. The stress shielding behavior of the interfaces is also found to be strongly dependent on the initial crack configuration, however, the coherent TT interface remains the most effective interface in terms of shielding in all cases.

MM 26: Topical Session: Hydrogen in Materials: from Storage to Embrittlement IV

Time: Tuesday 14:00–14:45 Location: C 130

MM 26.1 Tue 14:00 C 130

Accurate representation of hydrogen in metals by machine-learning enhanced modelling of nuclear quantum effects — •Kai Sellschopp[1], Thomas Klassen[1,2], Paul Jerabek[1], and Claudio Pistidda[1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon, Geesthacht, Germany — [2]Helmut-Schmidt-University, Hamburg, Germany

In a sustainable economy built on renewable energy, hydrogen plays a key role for storing energy and replacing fossil fuels. An efficient way to store hydrogen is to keep it in the solid state by binding it chemically in a metal hydride, which is particularly useful for seasonal energy storage or for applications where safety is a concern. Despite the fact that hydrogen is known to show nuclear quantum effects (NQE) even at higher temperatures, these have been neglected in computational studies of metal hydrides so far due to the high cost of path-integral molecular dynamics (PIMD) calculations. In this work, a machine-learned potential (MLP) is trained for the Mg-H system, a well-known hydrogen storage material, in order to speed up the simulations and bring down the cost. At the same time, the sample collection is accelerated by training the potential "on-the-fly" during classical molecular dynamics runs, where ab-initio calculations are replaced by the MLP whenever the estimated errors are low enough. In this contribution, I present the training and validation of this MLP and evaluate the speed-up that allows to perform computationally expensive PIMD calculations. First insights obtained from these calculations enhance our understanding of metal-hydrogen systems.

MM 26.2 Tue 14:15 C 130

Revised reaction-diffusion model of hydrogen trapping in cavities in metals — •Mikhail Zibrov and Klaus Schmid — Max Planck Institute for Plasma Physics, 85748 Garching, Germany

A reaction-diffusion model of hydrogen (H) trapping and release from a metal containing spherical cavities has been developed. The model uses a kinetic description of H atom trapping at the cavity surface and H_2 gas precipitation in the cavity volume. We show that the common assumption of a local thermodynamic equilibrium between H_2 gas in the cavity and the solute H is inadequate in several instances. We discuss the importance of correlated H retrapping by the same cavity and inhomogeneous H potential energy landscape in the vicinity of the cavity surface. H thermal desorption spectra from cavities have features that are difficult to describe with conventional models but are readily observed in experiments: Sharp rising edges of desorption peaks and constant desorption at a fixed temperature. The kinetics of H transport and trapping in the material containing cavities differs from that for point defects, especially at low temperatures.

MM 26.3 Tue 14:30 C 130

Hydrogen redistribution during electrochemical charging and mechanical testing: insights from a combined ab initio and finite element method — Christian Posch-Peperkorn[1], Philipp Hammer[1], Vsevolod Razumovskiy[1], Werner Ecker[1], Klemens Mraczek[2], Ali Tehranchi[3], and •Tilmann Hickel[4] — [1]Materials Centre Leoben Forschung GmbH, Austria — [2]voestalpine Stahl GmbH, Linz, Austria — [3]MPI für Eisenforschung Düsseldorf, Germany — [4]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

In advanced high strength steels the mechanisms of hydrogen embrittlement are expected to be strongly connected to the amount of retained austenite (RA) contained in the microstructure and its transformation upon deformation. We have developed a multi-scale model for the H redistribution during H charging and tensile loading within a martensitic/austenitic microstructure. Ab initio simulations have been used to resolve the complex energy profile of H in the phase boundaries. Representative microstructures with different amounts of RA have been converted form experimental SEM-EBSD measurements. Simulations with the finite element method (FEM) have been used to analyse H concentration profiles. The simulations confirm an accumulation of H within the austenitic phase during charging, which undergoes a phase transformation under mechanical load and releases accumulated H into the martensite matrix. The latter segregates to the microstructure regions subjected to high hydrostatic tensile stresses and plastic strains, driving H embrittlement.

MM 27: Data Driven Material Science: Big Data and Workflows IV

Time: Tuesday 14:00–14:45 Location: C 243

MM 27.1 Tue 14:00 C 243

A comprehensive screening of plasma-facing materials for nuclear fusion — •Andrea Fedrigucci[1], Paolo Ricci[1], and Nicola Marzari[1,2] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland

Plasma-facing materials (PFMs) represent one of the most significant challenges for the design of future nuclear fusion reactors. Inside the reactor, the divertor experiences the harshest material environment: intense bombardment of neutrons and plasma particles coupled with extremely large and fluctuating heat fluxes. The material chosen to cover this role in the fusion reactor ITER is tungsten. While no other material has shown the potential to match the properties of W, many drawbacks associated with its application remain. This work aims to produce a structured and comprehensive materials screening of candidate PFMs based on known crystal structures. The methodology to identify the most promising PFMs combines peer-reviewed data of inorganic crystals from the Pauling File database and first-principles DFT calculations of two key PFMs properties, namely the surface binding energy and the formation energy of a hydrogen interstitial. The materials that meet the necessary thermal performance to withstand heat loads are critically compared with the state-of-the-art literature, defining an optimal subset where to perform first-principles calculations. The majority of well-known PFMs - such as W, Mo, and carbon-based materials - are captured by this screening process, along with less familiar refractory materials that warrant further investigation.

MM 27.2 Tue 14:15 C 243

Machine learning modelling of local magnetic moments in Fe-based intermetallic compounds — •Bo Zhao[1], Kun Hu[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Peter-Grünberg-Str. 2, 64287 Darmstadt, Germany — [2]School of Materials Science and Engineering, Central South University, Changsha, 410083, Hunan, PR China

It is well known that the magnitude of magnetic moments is determined by the local crystalline environments as verified by studying the dimensional crossover behavior of a few representative systems such as Fe. To further generalise and quantify the mapping between the crystal environments and magnetic moments, we carried out machine learning modelling on Fe-based intermetallic compounds, with the corresponding magnitude of magnetic moments for Fe atoms varying between zero and four Bohr magneton (the atomic limit). Using the symmetry-adapted smooth overlap of atomic positions (SOAPs) as descriptors, it is observed that 2374 data for binary and ternary compounds collected from Materials Project are not sufficient for a reliable modelling. We further enriched the dataset by performing high-throughput calculations on Fe-(B, Co, Ti, Rh) binary intermetallic compounds, and the corresponding accuracy of the machine learning modelling is over 90% across all the systems. The results are further understood based on the Stoner model. Our work establishes a valid approach to model the physical properties dependent on the local crystalline environments.

MM 27.3 Tue 14:30 C 243

Synergistic catalytic sites in high-entropy metal hydroxide organic framework — Arkendu Roy, •Sourabh Kumar, Ana Guilherme Buzanich, Tilmann Hickel, Franziska Emmerling, and Biswajit Bhattachary — BAM, Bundesanstalt für Materialforschung und -prüfung, Richard-Willstätter-Str. 11, 12489 Berlin

Leveraging data-driven computational techniques accelerates catalytic process analysis and prediction, enabling materials discovery and chemical reaction optimization. Among such materials, high-entropy metal hydroxide organic frameworks (HE-MHOFs), with intricate structures surpassing conventional MOFs, are of special interest. In HE-MHOFs, high-entropy hydroxide layers are connected by ligands to form a superlattice, introducing structural disorder and diversity. Using the state-of-art ab initio calculations, the HE-MHOFs have been designed based on the stability of unary MHMOFs by constructing their ab initio Pourbaix diagram, followed by their synthesis using a conventional solvothermal process. The incorporation of different transition metals (TMs) alters the electronic structure, influencing adsorbate binding energy and catalytic activation potential. The SQS approach is used to deconvolute the atomic patterns and sample out the most favourable surfaces for OER investigations. Then the complexities in the proton-coupled electron transfer OER reaction mechanism are addressed by constructing a potential energy surface for each redox-active TM and comparing it to parent unary MOFs. A confirmation through in-situ XPS and EDX mapping complements our computational approach.

MM 28: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials I

Time: Tuesday 14:00–14:30 Location: C 230

MM 28.1 Tue 14:00 C 230

Structural and electronic properties of one-dimensional nanothreads derived from molecular precursors under pressure — •Samuel Vasconcelos and Michael Rohlfing — Institute for Solid-State Theory, University of Münster, Germany

Low-dimensional materials has been thoroughly investigated in the recent past decades. We focus mainly on one-dimensional materials, synthesized from molecular precursors. In particular, so-called nanothreads were presented in 2016 by Fitzgibbons et. al, derived from benzene molecules that were connected under pressure, changing their hybridization and remaining connected afterwards. Subsequently many other molecules were investigated, showing the same behaviour.

We discuss two cases, in which new properties are obtained under the same phenomenology of transformation. On the one hand, nanothreads derived from the porphyrin family presenting a metallic behaviour, which had not yet been observed in this class of materials. On the other hand, we present a new class of nanotubes with a sp3-connected carbon frame derived from the kekulene family, displaying a functional tubular character. Mechanical and electronic properties will be presented, as well as the basic formation mechanisms behind such transformations.

MM 28.2 Tue 14:15 C 230

New properties from 1D materials derived from molecules under pressure — •Samuel Vasconcelos and Michael Rohlfing — Universität Münster

Low-dimensional materials has been thoroughly investigated in the recent past decades. We focused mainly in the 1D materials. The precursor of a class in particular, the so-called nanothreads was presented in 2016 by Fitzgibbons *et. al*, when benzene molecules under pressure were connected, changing their hybridization and remaining connected afterwards. Subsequently many other molecules were investigated in order to obtain the same behaviour. We present two works, in which new properties were obtained under the same phenomenology of transformation. First, nanothreads derived from the porphirin family presenting a metallic behaviour, not yet observed in this class of materials. After we present a new class of sp^3 tubes derived from the kekulene family displaying a functional tubular character. Mechanical and electronic properties will be presented, and also the mechanisms behind such transformations are also exposed in these works.

MM 29: Poster II

Time: Tuesday 17:00–19:00 Location: Poster B

MM 29.1 Tue 17:00 Poster B

Exploring Mott Transition in the Hubbard Model using Slave Spin Mean Field Theory — •Youssra Anene — Cergy Paris Université, France

This poster delves into the application of the innovative slave spin mean field theory to investigate Mott transition within the single-band Hubbard model. The phenomenon of Mott transition, where a system transforms from a metallic to an insulating state, bears profound significance in the realm of condensed matter physics. Our study conducts an intricate analysis utilizing this novel theory to interpret the behaviors of crucial parameters, like quasiparticle weight, double occupancy within the Hubbard model. We examine how these parameters evolve with respect to the onsite Coulomb repulsion. The interpretations of resulting visual representations provide intricate insights into the dynamic intricacies of a Mott transition. Our inquiries are conducted under specific conditions: half filling (one electron per site), at absolute zero temperature, and in the context of a paramagnetic state. Through our work, we not only underscore the effectiveness of the slave spin mean field method in illuminating the fundamental mechanisms of the Hubbard model, but also outline potential paths for further exploration. We express our ambitions to extend this method to investigate the presence of Mott transition in other lattices . Additionally, we emphasize the potential application of this method to investigate the intriguing antiferromagnetic state within the Hubbard model and to explore the dynamics in the case of being out of equilibrium* .

MM 29.2 Tue 17:00 Poster B

RuNNer 2.0: An Efficient and Modular Program for Training and Evaluating High-Dimensional Neural Network Potentials — •Alexander L. M. Knoll[1,2], Moritz R. Schäfer[1,2], K. Nikolas Lausch[1,2], Moritz Gubler[3], Jonas A. Finkler[3], Emir Kocer[1,2], Alea Miako Tokita[1,2], Tsz Wai Ko[4], Marco Eckhoff[5], Gunnar Schmitz[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department of Physics, Universität Basel, Basel, Switzerland — [4]Department of NanoEngineering, University of California, San Diego, CA, USA — [5]ETH Zürich, Laboratorium für Physikalische Chemie, Zürich, Switzerland

Machine learning potentials (MLPs) have become a popular tool for large-scale atomistic simulations in chemistry and materials science. They provide efficient access to highly accurate potential energy surfaces (PES) generated from *ab initio* reference calculations. As methods in this field are becoming more and more complex and reach maturity, the development of efficient and user-friendly tools is increasingly important. We present the second major release version of RuNNer, an open source, stand-alone software package for the construction and evaluation of second-, third-, and fourth-generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 unifies the entire workflow in a fully MPI-parallel program: from the generation of atomistic descriptors, over the training of a specific machine learning model, to its final application in molecular dynamics.

MM 29.3 Tue 17:00 Poster B

Precise anisotropic thermal property measurement for AlAs/GaAs superlattice using Beam-Offset Frequency-Domain Thermoreflectance (BO-FDTR) technique — •ANKUR CHATTERJEE[1,2], D Dziczek[1], M Pawlak[1], and A Wieck[2] — [1]Institute of Physics, Nicolaus Copernicus University, Torun,Poland — [2]Chair of Applied Solid-State Physics, Ruhr-University Bochum

This description underscores the significance of effectively managing thermal conditions in high-performance semiconductor superlattice devices, specifically AlAs/GaAs superlattice with a period thickness of 52nm and a 50 nm Gold (Au) transducer on top. The focus of this work is on a detailed in-plane and cross-plane examination of thermal parameters, including thermal conductivity, thermal diffusivity, and thermal boundary resistance, within both single and multi-layered structures. This method utilizes rotating stages to precisely control the spatial separation (beam-offset3) between the pump-probe beam for in-plane thermoreflectance measurements. This non-contact pump-probe technique is purposefully crafted to measure thermal properties, encompassing cross-plane aspects3, across a broad frequency spectrum scanning from 10 Hz to 1.25 MHz. We found that measurements can be very precisely around 1-2% with expanded uncertainty (95% Confidence interval) whereas the standard error is 6-7% which is better compared to the previous work.

MM 29.4 Tue 17:00 Poster B

Using dynasor 2.0 for connecting simulation to experiment through correlation functions — •Esmée Berger, Erik Fransson, Fredrik Eriksson, Eric Lindgren, and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

The dynasor package is a flexible and efficient tool for calculating correlation functions, such as static and dynamic structure factors, both partial and total, as well as related current correlation functions. Analysis of these functions provides insight into the dynamics of a system, without the need for perturbative methods. Access to correlation functions allows for the direct prediction of experimental spectra by weighing the functions with cross sections (or form factors) of, e.g., neutrons, X-rays or electrons. Here, we show the wide variety of use-cases of dynasor, which has recently seen a major upgrade to version 2.0. Examples include static and dynamic structure factors, different experimental spectrum predictions, and phonon dispersions for a diverse set of systems.

MM 29.5 Tue 17:00 Poster B

Wannier orbital analysis: electronic structure characterization of transition metal diborides (TMB_2) by means of density functional theory — •Nebahat Bulut and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

Wannier orbital analysis is an efficient way for understanding the electronic structure of materials. This work focuses on the electronic properties of transition metal diborides(TMB_2), using Wannier functions to investigate the contribution of the orbitals to the electronic bands in these compounds. The results of our research offer information on the nature of chemical bonding and electronic interaction in TMB_2, investigating the influence of transition metal d-orbitals and boron sp-orbitals on the electronic energy and band structure. The computational methods were employed to obtain *maximally localized Wannier functions* (MLWF) using both **exciting-*fluorine*** and **Quantum Espresso** density functional theory codes. In addition, the findings may take the attentions for designing technological devices in the field of catalytic, semiconductors, hard coatings, and thermoelectric materials applications.

MM 29.6 Tue 17:00 Poster B

Electron-phonon interactions beyond DFT — •Aleksandr Poliukhin[1] and Nicola Marzari[1,2] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland

Electron-phonon interactions are vital in understanding materials' properties, including electron mobility and superconductivity. Accurate modeling of these interactions can lead to innovative applications, from efficient electronic devices to new superconducting materials. However, the limitations of traditional DFT in correct predictions of electronic structure properties necessitate the exploration of beyond-DFT functionals.

This study focuses on developing the framework for calculating electron-phonon matrix elements with any beyond-DFT functional that could provide information about eigenvalues and eigenfunctions of effective Hamiltonians, using as example hybrid and Koopmans functionals. We show the effects of more accurate electronic-structure treatments on both electron-phonon couplings and mobilities.

MM 29.7 Tue 17:00 Poster B

RIXS at the Oxygen K-Edge of Manganites — •Lukas Rump[1,2], Sreeju Sreekantan Nair Lalithambika[3], Simone Techert[1,3], Christian Jooss[1], and Peter E. Blöchl[1,2] — [1]Georg-August-Universität Göttingen — [2]Clausthal University of Technology — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg

Resonant Inclastic X-ray Scattering (RIXS) provides element specific information on both occupied and unoccupied states, and on two-particle excitations of the material. This spectroscopy technique correlates the emitted photons with the incident X-ray photons. Recent improvements in synchrotron radiation sources provide an energy resolution which allows for a detailed comparison with calculated spectra. In view of ongoing experimental investigations related to the oxygen evolution reaction in manganites we performed ab-initio first-principles calculations to explore the correlation of RIXS spectra with chemical processes.

We performed density-functional calculations of the manganite $La_{0.6}Sr_{0.4}MnO_3$. Calculated oxygen K-edge RIXS spectra yield good agreement with the high-resolution experimental results. The Mn-d orbitals are accessible to oxygen K-edge RIXS because of the delocalisation of Mn-d orbitals to the neighbouring oxygen sites. RIXS can be divided into direct and indirect processes. Direct processes can be described by the one-particle density of states. This enables the identification of experimental features originating from more intricate behaviour, such as core-hole interactions or additional excitation in the material.

MM 29.8 Tue 17:00 Poster B

modernization of the production of parts for a Russian combine — •Pavel Kartashev — Moscow, Russia

My graduation thesis was on the topic of optimization and modernization of the production of parts for a Russian combine, in which I conducted research, economic calculations, identified shortcomings and proposed a method of optimization, implementation of a new machine and equipment to replace human power with robotic power.

MM 29.9 Tue 17:00 Poster B

Computational modeling of mesoporous aluminosilicates via ab-initio based Machine Learning Interatomic Potentials — •Tom Schächtel, Jong-Hyun Jung, Konstantin Gubaev, and Blazej Grabowski — Institute for Materials Science, Department of Materials Design, University of Stuttgart, 70569 Stuttgart, Germany

Mesoporous silica are commonly used as catalyst supports for heterogeneous catalysis. To further enhance the properties of these materials the introduction of small amounts of metal atoms into the amorphous silica matrix was proposed. To better understand these mesoscale materials at the atomistic level a dual approach is suggested: The structure is obtained via Molecular Dynamics and Monte Carlo methods based on Machine Learned Interatomic Potentials, namely Moment Tensor potentials (MTPs), which are trained on Density Functional Theory data, while the electronic properties, specifically the electronic Density of States, is calculated with the Density Functional Tight Binding method. As a proof of concept a first trial MTP is trained to simulate the structure of a single mesopore contained in an amorphous aluminosilicate matrix. The accuracy of the trained MTP is investigated by analyzing the aluminum distribution and other properties of interest in a trial non-porous aluminosilicate bulk system containing additional hydrogen atoms.

MM 29.10 Tue 17:00 Poster B

Thermodynamic and kinetic study of Pt42.5CuxNi36.5-xP21 alloy variations — •Ziyu Ling[1], Maryam Chegeni[1], Ralf Busch[1], and Isabella Gallino[2] — [1]Chair of Metallic Materials, Saarland University, Germany — [2]Department of Materials Science and Engineering, Metallic Materials, TU-Berlin, Germany

In this work, the thermodynamic and kinetic properties of Pt42.5CuxNi36.5-xP21 (x = 36.5, 27, 18.25, 9.5, 0) glass-forming liquids are studied via Perkin Elmer DSC and Flash DSC (Mettler Toledo). The kinetic fragilities of the alloys are determined by measuring relaxation times in a broad heating rates range using a Tg shift method (Busch, 2000). In addition, the relaxation time of the deeply undercooled liquids is determined by FDSC via a step-response method (Monnier et al., 2020). Furthermore, the specific capacity heat (Cp) as a function of temperature for the glassy, liquid and crystalline state of the chosen alloys are determined. The thermodynamic fragility is assessed from the Cp difference between the liquid and crystalline states at the glass transition temperature and the driving force for crystallization is calculated using fitting parameters of thermodynamic functions. Moreover, the GFA of the alloy liquids is evaluated by determining their critical cooling rates and measuring their TTT-diagrams. The interfacial energy is obtained by JMAK fitting with TTT-diagrams. The aim of this work is to investigate the influence of Cu and Ni substitution on the thermophysical properties of the alloy and verify the argument that interfacial energy is the main contribution to the high GFA of Pt-P based alloys.

MM 29.11 Tue 17:00 Poster B

The first nanoseconds in the lifetime of a phase change material glass — •Jakob Ballmaier, Sebastian Walfort, and Martin Salinga — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Small volumes of so called phase change materials (PCMs) can be switched between a conductive crystalline state and high-resistance glass states. This property makes PCMs attractive for novel electronic memory devices, but there remain unresolved challenges. One issue for technical applications is the commonly observed resistance drift, i.e. the power-law-like increase in resistivity from microseconds up to years after the formation of the glass. Many different mechanisms have been proposed to explain this power-law behavior on the usually experimentally accessible time scales, for example by linking it to physical ageing.

On shorter time scales, capacitive currents can prevent accurate resistance measurements. Here we minimise capacitive currents by decoupling the excitation and probing mechanism. The nanoscopic PCM cell is melt-quenched with femtosecond laser pulses while continuously measuring the electrical resistance with a small, constant bias voltage. This measurement scheme allows us to resolve resistance drift from the first nanoseconds over 12 orders in magnitude in time. On short timescales we observe deviations from the well-known power-law behaviour. These observations may help to elucidate the mechanisms underlying resistance drift.

MM 29.12 Tue 17:00 Poster B

Experimental determination of material expansion upon hydrogenation of interstitial metal hydrides — •Gerd Stahlkopf — Hereon, Institute of HydrogenTechnology, Geesthacht, Germany

Hydride-forming materials (MH) are increasingly attractive since they provide efficient and safe hydrogen storage at mild temperatures and low pressures, offer a high volumetric storage density and are very interesting for stationary storage systems. Although the volumetric density of MH systems are relatively high, the MH-storage system needs to be optimized (maximum hydrogen storage capacity, efficient tank designs, longer system lifetime) and their practical application show relevant technological challenges. One of the main challenges for the application of MH as the storage medium is the resulting stress on the container walls when hydrogen is absorbed since the MH bed increases its volume by about 30 %. This "swelling" phenomenon is the bottleneck when designing a hydrogen storage system based on metal hydrides. Despite many efforts to avoid the by the swelling caused stress there is a lack of basic understanding of this swelling effect at the microscopic scale evolving upon the hydrogenation/dehydrogenation process over the cycles. This work focuses on the interdependency between the changing properties of the powder bed in- and ex-situ (e.g. particle size distribution, porosity, friction) and the stress caused by the swelling of MH over titration cycles. A deep understanding of the effect of powder bed parameters on the swelling stress will improve MH vessel designs and a proposed model. The changing characteristics of the MH-powders are investigated.

MM 29.13 Tue 17:00 Poster B

Reversion experiments for Guinier-Preston zones in Al-Cu — Max Obermair, •Hamideh Dorri, Johannes Berlin, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg

Both formation and dissolution of Guinier-Preston zones in Al-Cu alloys depend on the presence of excess vacancies. They are quenched in from the high temperature homogenisation treatment but will possibly disappear during the natural aging at ambient temperature. The lifetime of excess vacancies in pure Aluminium is much shorter than that in Al-Cu alloys, where vacancies presumably are trapped in GP zones. Loss of hardness during an increase in temperature to about 100°C after prolonged natural aging indicates a dissolution of the GP zones. Using hardness measurements, differential calorimetry and in-situ resistometry we were able to show, that this dissolution is still controlled by excess vacancies and that the formation of GP-2 zones depends on the thermal history of the samples.

MM 29.14 Tue 17:00 Poster B

Tuning magnetic properties in high entropy alloys by exploiting its anti-Invar properties — •Lennart Endler[1], Benedikt Eggert[1], Katharina Ollefs[1], Asli Çakir[2], Mehmet Acet[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Department of Metallurgical and Materials Engineering, Mugla University

Five or six-component high entropy alloys have been known in materials research for a long time and stand out due to their good mechanical properties [1]. CrMnFeCoNi, which has the same electronic configuration as fcc-Fe with an electron per atom ratio of $e/a = 8$, plays a crucial role here. Increasing the lattice constant in fcc-Fe changes the magnetic ordering from antiferromagnetic to ferromagnetic, which is also valid for CrMnFeCoNi [2]. Introducing interstitial carbon leads to a lattice expansion up to 0.02 Å [2]. Besides interstitial C, B can also be used to expand the volume of the lattice. Here, we investigate the effect of increasing interstitial C and B content on the structural and magnetic ordering by the combination of SEM, EDX, Mössbauer spectroscopy, XRD and magnetometry.

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[1] B. Schuh et al., Acta Mater. 96, 258 (2015)
[2] M. Acet, AIP Adv. 9, 095037 (2019)

MM 29.15 Tue 17:00 Poster B

Effects of relative-density ratio between upper- and lower-level structure in hierarchical nanoporous gold on mechanical behavior — •Hansol Jeon[1], Shan Shi[3,1], and Jürgen Markmann[1,2] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technol-ogy, 21073 Hamburg, Germany

Hierarchical nanoporous gold (HNPG), multiple-level structures, has receiving a lot of at-tention in application fields as one of new materials owing to higher surface area and faster reac-tivity compared to unimodal nanoporous gold (HNPG). Regarding its mechanical behavior, it has not been much research on this yet since it is quite advanced materials, and it would be expected to be more complex due to the multi-level's ligament sizes and relative densities. Here, we have investigated the effect of relative-density ratio between upper- and lower-levels on the mechanical properties of HNPG having the same total solid fraction by performing pillar compressive tests. HNPG samples having different ratio of relative density between upper- and lower-levels from the same precursor alloy Ag85Au15 by dealloying. The pillars were prepared by a focused ion beam (FIB), and compressive tests were conducted by a nanoindenter with a flat-punch tip. We have linked their mechanical properties with connectivity calculated from 3D reconstruction.

MM 29.16 Tue 17:00 Poster B

Composite Bipolar Plates for PEM Electrolysis — •Lindsay Lohmann, Maria Gaudig, and Ralf Wehrspohn — Martin Luther University Halle-Wittenberg, Institute of Physics, Group μMD, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany

Water splitting by PEM electrolysis (PEM: Proton Exchange Membrane) is a possible variant for the production of sustainable "green" hydrogen, however this process is currently too expensive and therefore uneconomical. Thereby, almost 50 % of the cost of the electrolysis cell and about 25 % of the total system costs are caused by one single component: the bipolar plate (BPP). Due to the electrochemical conditions prevailing in the fuel cell, only a few materials can be considered for the BPP. One of these materials is titanium. As this material is expensive in its pure form, titanium-polymer composites (with a high polymer content) are being researched as a possible alternative. We have already shown that composites with a titanium mass content of 80 % were able to meet the criteria (specified by the US Department of Energy) in the areas of electrical conductivity and mechanical stability. With a thin titanium coating, a better result can also be achieved in electrochemical corrosion. While such a BPP has been successfully incorporated into a PEM electrolysis cell and has been able to provide good electrolysis performance for short periods of time, the desired long-term stability has not yet been achieved. Further research and development in coating and surface roughness is therefore necessary. In this contribution we will present our current research results.

MM 29.17 Tue 17:00 Poster B

Multi-scale modelling and machine learning based simulation of the mechanical behaviour of graphite-resin composites — •Tobias Stegmüller — DLR, Institut für Test und Simulation von Gasturbinen, Am Technologiezentrum 5, 86159 Augsburg

To simulate the mechanical behaviour of a structural component it is important to link the microstructural features and properties of the construction material with its macroscopic shape and the acting forces. To achieve this we developed a multi-scale approach that constitutes of the following steps: First, the microstructure and its properties are collected by CT scans and mechanical tests, which are used to conduct FEM simulations of representative volume elements (RVE) that study the deformation behaviour. The response of the RVE is then homogenised over its volume and the homogenised properties are used for FEM simulations on the macroscopic length scale. Finally, the results of these simulations are used as training data for a machine learning algorithm, which is in the end capable of predicting the mechanical behaviour of structural components. The approach as well as its application to a graphite-resin composite are going to be presented.

MM 29.18 Tue 17:00 Poster B

Efficient Modelling and Synthesizability Descriptors of High-Entropy Ceramics — •Jacques Rene Eone II[1,2], Stefano Curtarolo[3], and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [3]Duke University, Durham, USA

High entropy materials have recently attracted significant interest due to their appealing mechanical, catalytic, and electronic properties. High-entropy ceramics consist of an ordered anion sublattice of carbon, nitrogen or oxygen and a disordered cation sublattice maximizing configurational entropy by randomly occupying it by five or more cation species (transition metal elements).

The reliable computational modelling of such systems can be realized by the partial occupation algorithm [1] implemented within the AFLOW software for materials design [2,3] by expanding the disordered system into a large set of ordered structures. These cells can then be treated by high-throughput *ab initio* calculations. For the actual realization of high-entropy materials, predictive synthesizability descriptors such as the entropy-forming ability (EFA) [4] are needed. We present here results on several high-entropy ceramic candidates, apply different synthesizability descriptors, and study their electronic and mechanical properties.

[1] K. Yang *et al.*, Chem. Mater. **28**, 6484 (2016).
[2] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[3] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[4] P. Sarker *et al.*, Nat. Commun. **9**, 4980 (2018).

MM 29.19 Tue 17:00 Poster B

Defects in magnesium and its alloys by atomistic simulation — •Hexin Wang[1], Julien Guénolé[2], Sandra Korte-Kerzel[1], Talal Al-Samman[1], and Zhuocheng Xie[1] — [1]Institut für Metallkunde und Materialphysik, RWTH Aachen University, Aachen D-52056, Germany — [2]Université de Lorraine, CNRS, Arts et Métiers, LEM3, Metz 57070, France

The properties of dislocation and grain boundaries in magnesium and its alloys were assessed by atomistic simulations employing various semi-empirical potentials. These results were compared with available experimental data and first-principles calculations. The mechanisms of <c> dislocation climb in Mg under c-axis tensile strain were investigated and correlated with the in-situ experimental observations. For grain boundary segregation, a strong correlation between the per-site segregation energies of alloying elements and the excess free volumes at grain boundaries was identified. The outcomes of this study provide insights into texture modification to inform the design of ductile magnesium alloys.

MM 29.20 Tue 17:00 Poster B

Precipitation role in strengthening and improved conductivity of HPTE-processed Al-Mg-Si alloy — •Vahid Tavakkoli, Andrey Mazilkin, Julia Ivanisenko, Christian Kübel, and Torben boll — Karlsruhe Institute of Technology, Karlsruhe, Germany

Aluminum alloys are attracting noticeable attention in electrical application due to their high conductivity, corrosion resistance and low price. However, low strength decreases their lifetime and subsequently results in significant expenses. Combination of SPD and post ageing is proposed as a potential approach to optimize electrical and mechanical properties . High pressure torsion extrusion (HPTE) is a relatively novel SPD method which can open up new possibilities for further scale-up the products size, as shown in this study. Samples processed via this method followed by post aging revealed high strength with markedly improved conductivity. Size, shape and density of precipitates are analyzed by means of HRTEM, STEM and APT.

MM 29.21 Tue 17:00 Poster B

An effective supramolecular Ni(II)-metallohydrogel based non-volatile memory device with excellent endurance — •Arpita Roy and Soumya Jyoti Ray — Department of Physics, Indian Institute of Technology Patna, Bihar-801106, India

Supramolecular gels are versatile materials that possess "smart" properties. They are used in various industries such as sensors, cosmetics, foods, nanoelectronics, logic gates and regenerative medicine. In this work, we have developed a well-organized and efficient method to rapidly synthesize a supramolecular metallohydrogel of Ni(II)-ion which is known as NiA-TA, has been established under ambient temperature and pressure. This metallohydrogel is prepared by using benzene-1,3,5-tricarboxylic acid as a low molecular weight gelator (LMWG) dissolved in DMF solvent at room temperature. Here, we have fabricated Schottky diode structures with a metal-semiconductor-metal geometry based on the nickel(II) metallogel (NiA-TA) to observe charge transport behavior. Remarkably, we have also developed NiA-TA based resistive random access memory1 (RRAM) device which shows bipolar resistive switching behavior at room temperature. This RRAM device shows an excellent ON/OFF ratio (˜110) which is measured from endurance test upto 5000 switching cycles. These structures hold tremendous potential for a wide range of applications, including non-volatile memory design, neuromorphic computing, flexible electronics, and optoelectronics device.

MM 29.22 Tue 17:00 Poster B

Computational elements based on coupled VO2 oscillators via tunable thermal triggering — •Guanmin Li, Zhong Wang, Yuliang Chen, Jae-Chun Jeon, and Stuart S. P. Parkin — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Computational technologies based on coupled oscillators are of great interest for energy efficient computing. A key to the development of such technologies is the tunable control of the interaction strength between the oscillators. Thus far, such coupled oscillators have been accomplished by additional external electronic components.

Here we show that the synchronization of closely spaced vanadium dioxide (VO2) oscillators can be controlled via a thermal triggering element that itself is formed from VO2. Thereby, we demonstrate the active tuning of coupled oscillation states between adjacent VO2 devices via a thermal cell that is placed between them. This tuning process allows the control of the amplitude, frequency and phase of the coupled VO2 oscillators. Moreover, we show that the net energy consumed by these oscillators is lower when their oscillatory states are coupled thermally than when they oscillate independently of one another. This frequency synchronization process is similar to the propagation of signals from pre-synaptic to post-synaptic neurons via the release of neurotransmitters. Our findings demonstrate that networks of thermally coupled oscillators allow for novel bio-inspired computational schemes.

MM 29.23 Tue 17:00 Poster B

Altering structure and optical properties of antimony without heat — •Julia Vehndel, Nils Holle, Sebastian Walfort, and Martin Salinga — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years phase change materials (PCMs) have attracted a lot of interest as electronic and photonic memory elements because of a high electrical and optical property contrast between crystalline and amorphous states. Switching between the two phases requires energy to allow the rearrangement of the atomic configuration. To this end the PCM is either heated moderately above the glass transition temperature to achieve recrystallization, or melted and rapidly quenched to form the disordered state. These thermal excitations entail significant energy costs in operating PCM-based memory.

In this study, we explore a more energy-efficient utilization of PCMs. We show that it is possible to achieve structural transformations by merely changing the occupation of electronic states in antimony, a single-elemental PCM. Using ab-initio simulations based on density functional theory, the resulting structural changes can be directly related to large alterations in optical properties in the visible and near-infrared region. Our results enable further research to elucidate the intricate coupling between structure and properties in these materials.

MM 29.24 Tue 17:00 Poster B

Exploring the atomic structure of Σ5 GBs in copper — •Hui Ding[1], Esakkiraja Neelamegan[2], Anoosheh Akbari[2], Sergiy Divinski[2], Gerhard Wilde[2], and Hui Ding[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]University of Münster, Münster, Germany

Grain boundaries (GBs) are material imperfections that have a strong influence on material properties. They can act as preferred diffusion pathways for solutes and hence impact the atomic transport properties of polycrystalline materials.

However, the relation between the atomic structure of GBs, possible deviations from the ideal structure, and their transport properties often remains unexplored. In this study, we employ aberration-corrected scanning transmission electron microscopy as a first step to characterize the atomic structure of a series of near-Σ5 (310) [001] symmetric tilt GBs.

While the kite-shaped structural units can be well-recognized in the Σ5 (310) [001] symmetric GBs, they also exhibit various defects, such as disconnections, asymmetric nanofacets, and secondary dislocations. These variations of the GB structure present an intriguing picture, particularly when considering their potential influence on the diffusion behaviour in the presence of deliberately introduced solutes. We will discuss the evolution of GB structure, the formation of GB defects and address their role on the kinetic properties of interfaces.

MM 29.25 Tue 17:00 Poster B

Nanoscopic electromagnetic field measurements in S/TEM — •Laura Niermann, Tore Niermann, Frederik Otto, Hüseyin Çelek, Simon Gäbel, Tolga Wagner, and Michael Lehmann — Technische Universität Berlin, Berlin

The electromagnetic properties of materials are governed by the microscopic electromagnetic fields that reside within them. In semiconductor functionality, examples range from static electric fields emerging due to a doping landscape, over hetero-interfaces between electrically polarized materials, to subtle microscopic responses to external electric or magnetic fields. Within the class of magnetic materials, the dynamic movement of domain walls is an example of this. (Scanning-) transmission electron microscopy (S/TEM) allows two complementary approaches to measure these nanoscopic fields. Both the deflection of an electron probe caused by the fields (differential phase contrast) or the phase shift of the electron waves caused by the electromagnetic potential (electron holography) can be measured quantitatively on a nanometer scale. Here we present current results of nanoscopic electromagnetic characterization, highlighting recent advances in understanding measurement artifacts caused by thin specimen surfaces, interactions with the electron probe, material contrasts and internal strain fields. In addition, novel approaches extend the measurements of electromagnetic fields to nanosecond timescales. We anticipate that these nanoscopic methods of electromagnetic field measurements have now been developed to such an extent that they can be used as a regular tool in solid state and material physics research.

MM 29.26 Tue 17:00 Poster B

Electron Beam Induced Currents: First Results from In-Situ Biasing S/TEM Experiments — •Kai-Luis Jakob, Santiago Koloffon, Frederik Otto, Hüseyin Çelik, Simon Gaebel, Tolga Wagner, Laura Niermann, Tore Niermann, and Michael Lehmann — TU Berlin

The main functionality of a plethora of electronic devices (e.g., solar cells or transistors) is based on p-n junctions, many of which are operated under an applied bias voltage. The behavior of such junctions in bulk material is well described by considering charge distributions at the interface. For thin samples, as one would typically investigate in a transmission electron microscope (TEM), these models break down as surface effects, such as preparation induced defects, become more dominant in comparison with a thin bulk core of such a sample. In this work, we show that contributions of the sample´s surface, such as enhanced electron-hole recombination probabilities, must be considered when observing electric devices in a TEM under bias. Furthermore, by comparing electron beam induced currents to nanometer scale measurements of carrier concentrations, both of which can be acquired simultaneously in a scanning transmission electron microscope, we demonstrate a pathway to future quantitative understanding of device behavior at such small scales under reverse bias.

MM 29.27 Tue 17:00 Poster B

In-situ/ Operando Electron Microscopy Characterization of model catalyst system for CO Oxidation — •Ajai Raj Lakshmi Nilayam[1], Carina Maliakkal[1], Ramin Shadkam[1], Nicola Da Roit[2], Di Wang[1], and Christian Kübel[1] — [1]Institute of Nanotechnology — [2]Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology (KIT)

In-situ scanning transmission electron microscopy (STEM) study of model catalyst systems with size selected Pt clusters on nanostructured CeO2 can be of aid to track the structure and morphological changes of clusters and to understand the chemistry during various pretreatment and CO oxidation reaction conditions. Pt clusters prepared by physical vapour deposition (cluster ion beam deposition (CIBD) on pulsed laser deposited CeO2) and wet chemical synthesis (polyol reduction to form Pt17 cluster followed by incipient wetness impregnation with CeO2 nanorods/ nanocubes) are of interests in this study. In-situ STEM study of CIBD deposited Pt200 on in-situ STEM nanoreactor chip (with SiNx membrane as support) resulted in cluster coalescence while imaging in vacuum and O2 and Ar environment at 100°C and higher, showing that the clusters are unstable on SiNx, whereas the clusters supported on CeO2 are more stable and agglomerate only at higher e- dose rates. In H2 atmosphere, the clusters on CeO2 are more stable, and do not coalesce even after prolonged exposure to e-beam at 300°C. This could be explained by Pt-mediated reduction of CeO2 overcoming the kinetic barrier for the reduction of CeO2.[1] References [1] Selim Alayoglu et. al., J. Phys. Chem. C 2013, 117, (50), 26608*26616

MM 29.28 Tue 17:00 Poster B

Thermal stability and mechanical properties of ultrafined grain CuZn alloy processed by HPT — •Yuting Dai[1], Marcel Sos[2], Torsten Scherer[1], Enrico Bruder[2], Karsten Durst[2], and Christian Kübel[1] — [1]Karlsruhe Institute of Technology, Institute of Nanotechnolog, Karlsruhe, Germany — [2]Technische Universität Darmstadt, Fachgebiet Physikalische Metallkunde, Darmstadt, Germany

Pure Cu undergoes instability after High-Pressure Torsion (HPT) processing. This investigation aims to explore the influence of solute elements on the mechanical properties, microstructure and thermal stability of CuZn5 and CuZn30 following HPT processing at room temperature.

CuZn5 and CuZn30 underwent high-pressure torsion press under 4.5 GPa for 25 turns to get saturated grain size. Isochronal heat treatment at various temperatures was applied to assess the thermal stability of these alloys. Automated Crystal Orientation Mapping (ACOM), providing comprehensive orientation maps at nanometer resolution, was employed to evaluate grain orientation, the fraction of high-angle grain boundaries, and average grain size.

Both CuZn5 and CuZn30 exhibit greater microstructural stability compared with Cu. Notably, CuZn5 maintains hardness after annealing at 200°C, whereas CuZn30 demonstrates annealing-induced hardening.

MM 29.29 Tue 17:00 Poster B

In situ nanotomography at P05 at PETRA III — •Silja Flenner[1], Malte Storm[1], Sandra Sefa[1], Johannes Hagemann[2], Sami Wirtensohn[1] und Imke Greving[1] — [1]Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, 21502 Geesthacht — [2]Deutsches Elektronen Synchrotron, Notkestr. 85, 22607 Hamburg

Nanotomography with hard X-rays has become a valuable tool in various field of research. The Helmholtz-Zentrum Hereon operates the nano branch of the imaging beamline P05 at PETRA III. The setup is optimized for in situ nanotomography studies and covers a wide range of applications, ranging from biological samples such as spider attachment hairs, wood and tissue, to bone implants, batteries, catalyst particles.

The nanotomography station offers transmission X-ray microscopy (TXM) as well as near- field holotomography (NFHT) covering absorption as well as phase contrast methods in an energy range of 8 to 17 keV. In the TXM, a spatial resolution down to 40 nm is achieved and allows for scan times of below one minute in the fast scan mode. The NFHT setup on the other hand offers low dose, quantitative phase contrast and a flexible magnification with even more extended space for in situ environments. In situ devices are available at the beamline such as nanoindentation, environmental control and micromanipulation such as force measurement and in situ wetting.

Thus, P05 is serving as an ideal probe for a wide range of length scales and applications, ranging from engineering over medicine to biology.

MM 29.30 Tue 17:00 Poster B

Fundamental studies of laser-polishing processes on polycristalline niobium — Florian Brockner, •Patrick Schwoche, and Dirk Lützenkirchen-Hecht — Bergische Universität Wuppertal

The interaction of intense pulsed- and CW-laser beams with metallic surfaces can be used to melt a near-surface region of the treated material for a short time, ideally leading to smoothed surfaces after cooling. In many cases, depending on the details of the laser treatment, periodic structures are observed on the surfaces of the irradiated materials. In particular due to its energy-efficient and flexible fabrication process and the resulting sub-wavelength periodic structures, there are many potential applications for laser polishing in the fields of materials processing, in particular for optics and mechatronics. However, a practical challenge for the laser treatments is the achievement of a homogenous and uniform surface after the procedure, because of the influence of local surface structures as e.g. polycrystalline materials feature grains of different size and crystallographic orientations, and the grain boundary regions further complicate the polishing. Here we will discuss the influence of the orientation of the laser polarization with respect to the crystallographic orientation of the grains at the surface and the presence of periodic surface structures, as well as their periodicity and amplitude. Investigations consist of a combined analysis with optical profilometry, scanning electron microscopy, and X-ray diffraction experiments.

MM 29.31 Tue 17:00 Poster B

A tale of two alloys: Extreme abnormal grain growth in AA5052 and AA5252 — •Karolína Gutbrod[1], Helmuth-André Schulz-Harder[1], Jules M. Dake[1], Madlen Atzen[1], Baptiste Flipon[2], Marc Bernacki[2], Timo Weihberger[3], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]MINES ParisTech, PSL University, France — [3]Speira GmbH, Hamburg, Germany

Grain growth is a phenomenon that occurs in polycrystalline materials during heat treatment. At a sufficiently high temperature, atoms located at grain boundaries can gain enough energy to hop from one grain to another, effecting a rearrangement of the microstructure. The grains that acquire additional atoms increase in size, while their counterparts shrink and eventually disappear, causing the average grain size to increase with time. If the grain size distribution maintains a unimodal shape during this process, we speak of normal grain growth (NGG). During another type of microstructural evolution – abnormal grain growth (AGG) – a few grains consume their neighbors, which enormously increases their size and cause a second maximum to appear in the grain size distribution. In most cases, the mechanisms responsible for AGG are still the subject of active debate. By investigating the occurrence of AGG in the Al-alloys AA5052 and AA5252, which differ only in their Cr content, we have attempted to contribute new findings to this discussion. Electron backscatter diffraction (EBSD) measurements – confirmed, in part, by diffraction contrast tomography (DCT) – point to similarities and differences in the conditions for AGG.

MM 29.32 Tue 17:00 Poster B

A journey from 2D into the third dimension of abnormal grain growth in the aluminum alloy AA5252 — •Helmuth-André Schulz-Harder[1], Karolína Gutbrod[1], Jules M. Dake[1], Madlen Atzen[1], Markus Ziehmer[1], Baptiste Flipon[2], Marc Bernacki[2], Pierre-Olivier Autran[3], Wolfgang Ludwig[3], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]MINES ParisTech, PSL University, France — [3]ESRF, France

The physics of grain growth are governed by thermodynamics. When the interface area between neighboring crystallites changes, the free energy F changes as well, which then acts as a driving force for the migration of grain boundaries. Under certain conditions, this can cause a subset of grains to start growing abnormally at the cost of neighboring grains. Although abnormal grain growth (AGG) has been investigated for decades, the underlying mechanisms are still not fully understood. We have investigated AGG in the aluminum alloy AA5252 using electron backscatter diffraction (EBSD), which is a 2D method. The results showed that the occurrence of AGG depends strongly on heating conditions, but because grain growth is a three-dimensional process, only 3D investigations can give a complete picture of the process. Therefore, diffraction contrast tomography (DCT) and phase contrast tomography (PCT) measurements were performed with synchrotron radiation to obtain 3D time-resolved datasets of microstructural evolution and insight into the role played in AGG by second-phase particles.

MM 29.33 Tue 17:00 Poster B

Oxygen-surface interactions investigated by atomistic simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer energy by various mechanisms and, due to their high chemical reactivity, may form oxides. This project aims to investigate atomic oxygen-metal and atomic oxygen-oxide interactions on an atomistic level using molecular dynamics simulations and density functional theory based calculations. The fraction of reflected and adsorbed atoms and the energy and momentum transfer will be determined depending on the material, incidence energy, incidence angle, surface roughness, and surface temperature. A focus lies on the mechanisms of energy loss and chemical reactions at the surface. Furthermore, adsorption energies and diffusion paths of oxygen at the surface, within the bulk, and along metal-oxide interfaces will be calculated. In a long-term perspective, we will deliver, in cooperation with project partners, an overall validated methodology for the calculation and provision of a database of atomic oxygen-surface interactions under relevant VLEO conditions.

MM 29.34 Tue 17:00 Poster B

Formation and functionalities of self-assembled monolayers on nanoporous gold — •Eva-Maria Steyskal[1], Elisabeth Hengge[2], Lara Novak[1,2], and Roland Würschum[1] — [1]Institute of Materials Physics, NAWI Graz, Graz University of Technology, Austria — [2]Institute of Biotechnology and Biochemical Engineering, NAWI Graz, Graz University of Technology, Austria

Self-assembled monolayers (SAMs) are a popular strategy for surface functionalization of electrodes, yet hardly studied for defect-rich or porous materials. Here we give an overview of our group's systematic work on the SAM-functionalization of nanoporous gold (np-Au) obtained by electrochemical dealloying. Via in-situ resistometry, the different stages of the SAM formation process in the porous structure can be clearly distinguished [1].

As specific examples of SAM functionalities, we demonstrate electrochemical controllability of the surface charge [2], which is even superior on np-Au compared to planar electrodes, as well as a sensing application, namely the detection of fluoride ions in water [3], which relies on a SAM with a boronic acid functional group.

This work was financially supported by the Lead Project (LP-03) Porous Materials @ Work for Sustainability at TU Graz as well as the Austrian Science Fund FWF (P36409).

[1] E. Hengge et al., Beilstein J. Nanotechnol., 2019, 10, 2275-2279, [2] E. Hengge et al., Phys Chem Chem Phys, 2021, 23, 14457-14464, [3] L. Novak et al., RSC Adv., 2023, 13, 6947-6953

MM 29.35 Tue 17:00 Poster B

Metavalent bonding: A universal strategy to enhance the thermoelectric performance of GeSe alloys — •Xin Zhong, Yuan Yu, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074, Aachen, Germany

Generating electricity in a sustainable and environmentally friendly manner is currently a topic of great concern. Thermoelectric materials, capable of directly converting heat into electricity through temperature differences, provide an effective means to harness waste heat. Doping is a practical approach to enhance thermoelectric properties, even for materials with initially poor thermoelectric performance, such as GeSe. Previous studies have demonstrated that the successful doping effects in GeSe can only be enabled by forming a metavalently bonded phase. Effective dopants such as $AgSbSe_2$ and $AgBiTe_2$ that can enable such a chemical bonding transition of GeSe from covalent to metavalent are confined in a special region of a map, where metavalently bonded compounds prevail. Yet, the universality of this concept has to be verified. Here we select PbTe from this metavalent region to alloy with GeSe.

We prove that a new metavalently bonded GeSe phase can be formed with proper contents of PbTe alloying using atom probe tomography, optical property measurements, and density functional theory calculations. The resulting metavalently bonded alloy shows greatly improved thermoelectric performance by a factor of more than ten. We prove that such metavalent bonding can be a universal strategy for designing high-performance chalcogenide thermoelectrics.

MM 29.36 Tue 17:00 Poster B

Investigation of fatigue-generated vacancies in thin metal films using nanoindenter creep tests — •My Nguyen, Jan Verhoeven, Thomas Brede, Dominik Tönnies, and Cynthia A. Volkert — Institute for Material Physics, Georg-August University of Göttingen, Germany

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 by using delay line structures (with thin copper films on top) on which standing surface acoustic waves (SAW) are generated. Contributions from thermal drift during the creep tests have been minimized using a continuous stiffness measurement (CSM) method. The results confirm that using the developed method, it is possible to perform highly reproducible measurements. Turning the SAW loading on and off induces changes in raw displacement depth data which consistently correlate with the applied power. The CSM-corrected data also show SAW-induced changes, although not always assigned to creep behavior, but might be caused by the presence of artifacts and other effects. Initial interpretations of these variations regarding the different samples can be provided by the ellipsoidal concept of surface waves and tip asymmetry.

MM 29.37 Tue 17:00 Poster B

Phase transformation in the Palladium Hydrogen system: Effects of boundary conditions and stress relaxation on phase stabilities — •Stefan Wagner[1], Alexander Dyck[2], Astrid Pundt[1], and Thomas Böhlke[2] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Institute of Engineering Mechanics (ITM), Karlsruhe, Germany

The thermodynamic stability of phases in alloys undergoing structural phase transitions can be modified by constraints. Utilizing palladium-hydrogen as a model, within a linear-elastic chemo-mechanical approach we study modifications of the system's Helmholtz free energy and chemical potential upon different constraints. The palladium-hydrogen system decomposes into a solid solution phase and a hydride phase at critical conditions. Depending on the chosen elastic boundary conditions systematic variations of the driving force for hydride formation in temperature-concentration space are revealed.

In real systems plastic deformation can occur, when critical energy densities of the alloy are reached upon elastic straining. Plastic deformation is shown to strongly reduce the stability of the palladium-hydrogen solid solution phase on the expense of eased hydride formation.

MM 29.38 Tue 17:00 Poster B

Interaction of reactive Fe-nanoparticles with the intermetallic compounds (IMC) layer during reflow soldering solidification — •Farzad Khodabakhshi[1,2], Irina Wodak[1], Andriy Yakymovych[1], Gerhard Wilde[2], and Golta Khatibi[1] — [1]Institute of Chemical Technologies and Analytics, Vienna University of Technology, Getreidemarkt 9/164, A-1060 Vienna, Austria — [2]Institute of Materials Physics, University of Münster, Münster, 48149, Germany

As an innovative idea, reactive iron nanoparticles were applied at the interface between Sn-Ag solder alloy and copper substrates and mixed with the flux. To this end, the hindering effect of such nanoparticles against the intermetallic compound*s (IMC) layer growth during the reflow solidification in reactive soldering was revealed to be very significant in improving the functional performance of the solder joints. The leading focus of the present research is on the characterization of the interaction between the Fe-nanoparticles and the IMC layer using advanced microscopy techniques. In this case, the focused ion beam (FIB) technique was applied to prepare thinned lamellae from the head of the IMC layer interface with the solder joint area, followed by scanning transmission electron microscopy (STEM) observations and analyses of nano-scale precipitates through the IMC layer. Interestingly, the nano-scale features exhibited in situ phase transformations inside the Cu6Sn5 solder alloy layer due to iron diffusion and decomposition by solid/liquid edge migration and involved reactions.

MM 30: Invited Talk: Anna Kareer

Time: Wednesday 9:30–10:00 Location: C 130

Invited Talk MM 30.1 Wed 9:30 C 130

Scratching the surface: understanding plasticity associated with microscale asperity contacts — •Anna Kareer — Department of Materials, University of Oxford, Oxford, United Kingdom

When considering macroscale wear, an understanding of the effect of plasticity is essential; plastic behaviour directly affects the macroscopic wear processes and provides a quantitative mechanism of energy dissipation in friction. It is well established that macroscale friction and wear behaviour is controlled by micronmeter sized surface asperities, thus, understanding and predicting wear relies on a mechanistic understanding of the plastic deformation associated with a micronmeter sized sliding asperity. In this work we use nanoscratch testing to probe microscale deformation from a frictional contact in metallic samples, in an attempt to understand the mechanisms of deformation associated with a single sliding asperity. Nanoscratches are made using a nanoindenter operating in force-controlled mode and the displacement is monitored throughout the experiment. The localised deformation is characterised using advanced microscopy, both at the surface and subsurface. A physically based crystal plasticity finite element model (CPFEM) is used to simulate the deformation and provides insight into the 3D evolution of the deformation fields surrounding the nanoscratch experiment, as it transitions from a statically loaded indent to a kinetic scratch. Furthermore, in-situ high temperature nanoscratch experiments reveal the sliding deformation behaviour of materials operating at elevated temperatures, where in service, macroscale wear phenomenon are often accelerated.

MM 31: Topical Session: Hydrogen in Materials: from Storage to Embrittlement V

Time: Wednesday 10:15–11:30 Location: C 130

Topical Talk MM 31.1 Wed 10:15 C 130

Compositional effects on the hydrogen sorption in refractory high entropy alloys — •Claudia Zlotea and Nayely Pineda-Romero — ICMPE CNRS Thiais France

High entropy alloys represent a novel alloying strategy that can yield exceptional performance properties needed across a variety of technology applications, including hydrogen storage. Examples include high volumetric capacity materials (BCC alloys forming FCC dihydrides) with improved thermodynamics relative to conventional high-capacity metal hydrides (like MgH2), but still further destabilization is needed to reduce operating temperature and increase materials-level capacity. In this presentation, we will show a strategy to effectively destabilize TiVNb-based hydrides by adding small amounts of Al/Mo/Cr. We specifically evaluate the effect of Al/Mo/Cr addition on the phase structure, microstructure, hydrogen absorption and desorption properties. The experiments demonstrate that increasing Al/Mo/Cr content results in a significant hydride destabilization. The change of the local structure as function of chemical composition and hydrogen concentration will be emphasized by total X-ray scattering at synchrotron and related pair distribution function analysis. Moreover, the phase transition during reaction with hydrogen will be highlighted by in situ neutron and synchrotron X-ray diffraction. Finally, hydrogen absorption/desorption cycling properties will be addressed with an emphasis on the structure/microstructure cycle-life stability. The presentation will conclude about possible strategies for the design of high-entropy hydrides targeted for specific hydrogen use cases.

MM 31.2 Wed 10:45 C 130

Revealing hydrogen-rich phases in NiTi shape memory alloys — •David Holec[1], Anna M. Paulik[1], Adam Weiser[2], Juraj Todt[1], Jitka Holcova[1], Jozef Keckes[1], and Antonin Dlouhy[2] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Institute of Physics of Materials ASCR, Zizkova 22, 616 62 Brno, Czech Republic

The shape memory alloy NiTi is particularly popular for medical applications and implants due to its excellent biocompatibility and corrosion resistance. Specifically, the interaction with hydrogen is critical due to its natural prevalence in living tissues.

The focus of this work is the characterization of NiTi hydrides using the density functional. Based on experimental observations, structural models have been created for different hydrogen concentrations and distributions. The formation energy has been calculated and compared between the models to find the most stable hydride structure. This is further complemented using Monte Carlo optimization of interstitial H distributions, using DFT-derived ML interatomic potential. The thus obtained compositional dependence of structural parameters is used to rationalize observed variations in the B2 and B19* lattice parameters and associated volumetric changes obtained from the insitu X-ray synchrotron diffraction measurement during the H uptake experiment.

MM 31.3 Wed 11:00 C 130

Mixed Metal Solid Solutions in Amide-Hydride Systems — •Thi Thu Le[1], Michele Chierotti[2], Stefan Walders[3], Denis Kramer[3], Alexander Schoekel[4], Thomas Klassen[1,3], and Claudio Pistidda[1] — [1]Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — [2]University of Torino, Torino, Italy — [3]Helmut Schmidt University, Hamburg, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Metal amide-hydride materials have been extensively studied for use in energy applications. In particular, the solid solution formation in metal-amide hydride system promotes fast hydrogen sorption kinetics and tunes the thermodynamics, which allow hydrogen absorption/desorption below 150 *C in hydrogen storage systems. In addition, these intermediates are potentially ionic conductors for solid-state batteries. In this work, a series of M-N-H solid solution structures based on mixed MNH2-MH materials of Group 1 elements (M = K, Rb, Cs and their combinations) is reported. The results obtained by ex-situ / in-situ XRD, and MAS NMR confirm the formation of mixed solid solution associated with an exchange between both anionic (NH2- and H-) and cationic species (K+, Rb+ and Cs+). Moreover, MD calculations show that the NH2 rotation barrier is lowest in the Cs system, which has the lowest phase transition temperature, indicating a positive correlation of two variables, where a higher anion rotation barrier is associated with a higher phase transition temperature, in agreement with experimetal data. This work provides the basis for further studies on the ionic conductivity of solid electrolytes or dopants.

MM 31.4 Wed 11:15 C 130

Hydrogen storage in porous FeTi nanofoams — •Lukas Schweiger[1], Florian Spieckermann[1], Nikolaos Kostoglou[1], Sebastian Stock[2], Peter Cengeri[3], Michael Zehetbauer[3], Oskar Paris[2], Daniel Kiener[1], and Jürgen Eckert[1,4] — [1]Montanuniversität Leoben, Department Materials Science, Austria — [2]Montanuniversität Leoben, Chair of Physics, Austria — [3]University of Vienna, Faculty of Physics, Austria — [4]Austrian Academy of Sciences, Erich Schmid Institute, Austria

While metal hydrides are promising for hydrogen storage, challenges persist due to slow kinetics, inadequate stability, and unfavorable pressure-temperature conditions. A well-studied material is the intermetallic FeTi, qualifying as a good candidate to overcome these limitations. We intend to achieve this by prototyping a FeTi-based nanoporous metallic foam. Therefore, FeTi and Cu powders were blended, whereby Cu is removed after high-pressure torsion (HPT) processing. Detailed exploration of the FeTi-Cu system, including varying deformation temperature and Cu content, reveals optimal conditions for obtaining a homogeneous nanocrystalline composite. The process retains flexibility, providing tunability through temperature adjustments during HPT or subsequent heat treatments. Removing the Cu transforms the nanocomposite into a metallic nanofoam. Characterization via nitrogen ad-/desorption highlights a specific surface area of 17 m2/g and a well-defined mesoporous structure. Hydrogen absorption measurements reveal rapid and reversible hydrogen uptake, with the nanoporous FeTi maintaining mechanical stability.

MM 32: Developement of Calculation Methods I

Time: Wednesday 10:15–11:30 Location: C 243

MM 32.1 Wed 10:15 C 243

Insights into Modelling Silica Aerogels: A Computational Approach — •Prakul Pandit[1], Nina Borzecka[1], and Ameya Rege[1,2] — [1]Institute of Materials Research, German Aerospace Center, Cologne, Germany — [2]School of Computer science and Mathematics, Keele University, Staffordshire, England

In recent years, extensive research has focused on comprehending the structure-property relationships of silica aerogels, aiming to tailor their characteristics for specific applications. Several computational studies describing the network formation in these aerogels have been reported, primarily methods based on the Brownian motion of particles. However, these studies simplify the morphology by assuming monodisperse particles and representing the Brownian motion with a singular numerical parameter of particle step size. Additionally, the gelled structure is assumed to represent the final dried structure. In this study, we introduce a model to emulate the gelation kinetics and material behaviour of silica aerogels. Notably, the model incorporates the polydispersity observed in experimental setups, thereby offering a robust depiction of morphology based on experimentally observed condensation kinetics. A pivotal improvement involves correlating model numerical parameters with experimental data to accurately emulate the physical kinetics of the gelation. Furthermore, we utilise finite element methods to analyse the volumetric contraction experienced by the gelled system during and post-drying. Thus, the model aims to present a better computational understanding of silica aerogels, that is both more precise and representative.

MM 32.2 Wed 10:30 C 243

Simulation of properties of anisotropic porous ceramics based on 3D reconstructed microstructures — •Radu Stefan Stirbu[1], Leontin Padurariu[1], Vlad Alexandru Lukacs[1], Fereshteh Falah Chamasemani[2], Roland Brunner[2], and Liliana Mitoseriu[1] — [1]Dielectrics, Ferroelectrics & Multiferroics Group, Faculty of Physics, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania — [2]Department Materials Center, Leoben Forschung GmbH, Leoben A-8700, Austria

The functional properties of electroceramics are strongly dependent on their porosity level, as well as on the microstructural characteristics of the existing pores (size, shape, orientation, distribution, connectivity). In the present work, the dielectric, ferroelectric and piezoelectric properties of porous BaTiO3 ceramics with anisotropic porosity are numerically estimated by using Finite Element Models, with realistic geometrical input, based on X-Ray tomography data. By this method, peculiar features as structural defects, cracks, percolated pores can be locally investigated and their role on the material property failure can be better understood. Further, the dielectric, ferroelectric and piezoelectric properties are estimated and compared to the experimental ones. The employed approach provides a bridge from meso- to macroscale in understanding the relationship between the microstructure and material properties.

MM 32.3 Wed 10:45 C 243

Full anharmonicity of transition states via ab initio machine-learning: Self-diffusion in tungsten — •Blazej Grabowski[1], Xi Zhang[1], and Sergiy Divinski[2] — [1]Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany

We propose an efficient ab initio framework to compute the Gibbs energy of the transition state in vacancy-mediated diffusion including the relevant thermal excitations at density-functional-theory level. With the aid of a bespoke machine-learning interatomic potential, the temperature-dependent vacancy formation and migration Gibbs energies of the prototype system body-centered cubic (BCC) tungsten are shown to be strongly affected by anharmonicity. This finding explains the physical origin of the experimentally observed non-Arrhenius behavior of tungsten self-diffusion. A remarkable agreement between the calculated and experimental curvature of the temperature-dependent self-diffusivity is revealed. The proposed computational framework is robust and broadly applicable, as evidenced by first tests for a hexagonal close-packed (HCP) multicomponent high-entropy alloy. The successful applications underscore the attainability of an accurate ab initio diffusion database.

Zhang, Divinski, and Grabowski, arXiv:2311.00633 (2023).

MM 32.4 Wed 11:00 C 243

Simulation of hot carrier generation and distribution in large plasmonic nanoparticles — •Simão João, Hanwen Jin, and Johannes Lischner — Department of Materials, Imperial College London

Energetic or hot carriers in metallic nanoparticles are generated from the decay of the localized surface plasmon via the Landau damping mechanism and can be harnessed for applications in photocatalysis or sensing. A detailed understanding of hot-carrier properties and their dependence on the nanoparticle size, composition, environment and shape is needed to optimize devices. However, standard electronic structure methods, such as those based on first-principles density-functional theory, cannot be applied to nanoparticles of experimentally relevant sizes. To address this challenge, we use a recently developed approach that combines an atomistic tight-binding description of the nanoparticles with a Chebyshev decomposition of Fermi's golden rule in order to calculate the rate of hot carrier generation and the spatial and energetic distribution of electrons. This opens up the possibility of simulating nanoparticles with millions of atoms. We will present results for gold nanoparticles of different shapes including cubes, octahedra and dodecahedra and discuss their potential for the photocatalytic reduction of CO2 into high-value chemicals.

MM 32.5 Wed 11:15 C 243

Detecting vacancy defects in graphene nanoribbon: a Floquet-Bloch formalism — Gulshan Kumar, Shashikant Kumar, and •Prakash Parida — Department of Physics, Indian Institute of Technology Patna, Bihta, Patna, India

We prescribe a theoretical approach aimed at predicting the spatial position of monovacancy defects within zigzag graphene nanoribbons (ZGNRs) at edges. Our methodology involves a comprehensive study of the Floquet quasi-energy band structure, specifically under the illuminating influence of circularly polarized light. Notably, our findings reveal that the strategic placement of monovacancy defects at edges in ZGNRs possesses remarkable potential in regulating the influential flat band edge state in the quasi-energy spectrum. These fascinating properties and findings can be harnessed and applied for various practical applications, further highlighting the significance and relevance of our theoretical framework.

MM 33: Transport in Materials: Diffusion, Conduction of Charge or Heat III

Time: Wednesday 10:15–11:30 Location: C 264

MM 33.1 Wed 10:15 C 264

Correlation of structural changes and hydrogen diffusion in polycrystalline WO$_3$ thin-films by combining in situ transmission measurements and Raman spectroscopy — •Tim K. Hecker, Markus S. Friedrich, Alexander G. Strack, Paul Tuchecker, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

To better understand hydrogen diffusion in tungsten trioxide thin films, such samples were microstructured with a PMMA film in such a way that the contact surface with the electrolyte is limited to a narrow stripe-like gap. This allows us to study the lateral diffusion of hydrogen under the PMMA film, increasing the analysable path and time scale by several orders of magnitude and thus significantly improving the spatial and temporal resolution of in-situ transmission and Raman measurements. Spatially resolved transmission measurements in the wavelength range of 633±55 nm show that the investigated diffusion is dependent on the hydrogen concentration. Time-resolved Raman measurements with a 633 nm laser at different distances from the electrolyte contact area show that the transition between the two diffusion coefficients is characterised by a phase transition of the crystal structure to higher symmetry. The results are also supported by a spatially and temporally resolved diffusion simulation. In addition, the measurement method presented here is universally applicable.

MM 33.2 Wed 10:30 C 264

Intermixing of nanoparticle metal alloy — •Yong Li[1] and Jörg Weissmüller[2,1] — [1]Institute of HydrogenTechnology, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Metal or its alloy nanoparticles are widely used in catalysis. In this study, the surface diffusion-dominated Brownian motion of nanoparticles at different temperatures is simulated using Kinetic Monte Carlo (KMC). The initial structure of nanoparticles are ordered FCC binary alloy with radii ranging from 2 to 8 nm. It is found that the displacement of the particle centre of mass, R_{cms}, scales with time, t, as $R_{\mathrm{cms}} \propto \sqrt{Dt}$. The diffusion constant, D, has a power law relationship with the particle radius, r, $D \propto r^{-4}$. The Cowley short-range ordering parameter, α_1, is detected for the first nearest-neighbor shell. The time of α_1 evolves to half of its initial value, $t_{\frac{1}{2}\alpha_1}$, shows a power-law dependence to r with a scaling exponent of 6.

MM 33.3 Wed 10:45 C 264

Interdiffusion in Cu-Ni couples with end-members severely plastically deformed via high-pressure torsion — •Esakkiraja Neelamegan[1], Jasper Berndt[2], Stephan Klemme[2], Gerhard Wilde[1], Aloke Paul[3], and Sergiy. V Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster-48149 Germany — [2]Institute for Mineralogy, University of Münster, Münster-48149 Germany — [3]Department of Materials Engineering, Indian Institute of Science, Bangalore-560012 India

For coarse-grained polycrystalline alloys, interdiffusion of the Cu-Ni system is investigated, and the composition-dependent interdiffusion coefficients are known to decrease with an increase in the Ni concentration. The present study explores the influence of the end members' microstructure state on the interdiffusion behaviour. Severe plastic deformation via high-pressure torsion is used. We estimate the composition-dependent tracer diffusion coefficients using the augmented tracer-interdiffusion couple approach. The interdiffusion behaviour of undeformed (coarse-grained) and deformed (ultra-fine-grained) materials are compared. An anomalous diffusion behaviour with respect to the annealing temperature is observed. The comprehensive tracer and interdiffusion data shed light on the impact of plastic deformation on the interdiffusion behaviour.

MM 33.4 Wed 11:00 C 264

Impurity diffusion measurement in liquid Al based alloys using X-ray Radiography — •Masato Shiinoki[1], Elke Sondermann[1], and Andreas Meyer[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institute Max von Laue - Paul Langevin (ILL), 38042 Grenoble, France

The high accuracy measurements of the impurity diffusion coefficient in liquid metals are indispensable for modeling diffusion theories. The aim of this study is to investigate how the difference in impurity diffusion coefficient in liquid Al is expressed by the hard-sphere model. The impurity diffusion coefficients in liquid Al were measured using the in-situ shear cell method with X-ray radiography technique at 973, 1020, and 1060 K. The concentrations of the two parts of the diffusion couple were chosen to be pure Al and 5 at% Cu, 1 at% Sn, 1 at% Au, 1 at% Ag, and 0.8 at% Bi in Al. The diffusion process was started at connecting each interdiffusion couple after shearing the furnace and concentration profiles were obtained every second. The impurity diffusion coefficients were calculated from the linear fittings to the mean square diffusion distance which is derived from the concentration profiles using Ficks law. The results showed that the excess entropy model using hard sphere reproduced the measured impurity diffusion coefficients in liquid Al better than the hard-sphere model derived from Enskog theory. This excess entropy model reproduces the impurity diffusion coefficients better for other temperatures as well by considering the temperature dependence of the packing density.

MM 33.5 Wed 11:15 C 264

Simulation of Dendrite Growth at the Electrode Interface in Lithium Metal Batteries — •Len Kimms[1], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz Institute Münster (IEK-12), Ionics in Energy Storage, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster

In this talk, we will present a simulation study that investigates the formation and growth of dendrites. The limitations of current commercial battery technologies can be possibly solved by using metallic lithium as electrode material. Lithium metal batteries (LMB) employ lithium metal anchored on a current collector as negative electrode. When charging the battery, cations are reduced at the electrode interface. Controlling the deposition to favor uniform plating is inherently challenging. The high reactivity of lithium metal can form a solid electrolyte interphase (SEI) which together with electric–field effects and a locally varying composition of the electrolyte drive dendritic deposition. A generic coarse–grained model is employed to investigate fundamental driving forces on the dendrite morphology. Not only electric–field effects, transport in the electrolyte, and cation concentration can be evaluated but also the optimization of more intricate procedures is possible. The model allows the exploration of dendrite–suppression techniques like pulse charging, application of an artificial SEI layer, or host structures on the electrode. To understand the complex interplay between microscopic electrochemical conditions, the model may be augmented by insights from molecular dynamics simulations.

MM 34: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials II

Time: Wednesday 10:15–11:30 Location: C 230

MM 34.1 Wed 10:15 C 230

influence of spinodal decomposition on mechanical properties and oxidation resistance of self-passivating WCrY alloy (SMART) for a fusion power plant — •Jie Chen[1], Elena Tejado[2], Andrey Litnovsky[1], Jesus Gonzalez-Julian[3], and Martin Bram[1] — [1]Forschungszentrum Jülich GmbH - Institut für Energie- und Klimaforschung, D-52425 Jülich, Germany — [2]Universidad Politécnica a de Madrid - Departamento de Ciencia de Materiales-CIME. E-28040 Madrid, Spain — [3]RWTH Aachen University - Institute of Mineral Engineering, 52074 Aachen, Germany

Self-passivating Metal Alloys with Reduced Thermo-oxidation (SMART) with a composition of W-11.4wt%-0.6wt%Y is considered as a promising plasma-facing material in fusion power plants. In the present work, the as-sintered SMART material, fabricated via ball milling and field-assisted sintering, is annealed at 1000°C for different amount of time to trigger spinodal decomposition. With 100 hour annealing, the material is characterized by submicron Cr-rich phases with 69.2at% Cr and W-rich matrix phase. The 100h-annealed alloy is significantly softened (HV1011) compared to the as-sintered state. The three point bending tests have been done from room temperature up to 1100°C and it is found that annealed specimens show both higher strength and fracture toughness at all tested temperatures. The oxidation resistance of annealed samples has also been investigated at 1000°C under synthetic air with 70% relative humidity. Details of the work will be given in this contribution.

MM 34.2 Wed 10:30 C 230

Investigation of Age-Hardened AlCu Alloys with Coincidence Doppler Broadening Spectroscopy — •Leon Chryssos and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

The positron in matter acts as a defect sensitive probe. Coincidence Doppler Broadening Spectroscopy (CDBS) is sensitive to open volume defects and to the elemental signature at the positron annihilation site. In contrast to other positron annihilation techniques, this enables the analysis of vacancy-solute complexes in solids and precipitates in the host matrix. In age-hardened AlCu alloys Cu-rich clusters are responsible for a significant improvement of the strength of the material. In this presentation, CDBS was used to investigate the Cu cluster formation in such alloys, especially after solution annealing and quenching. Combined with our new analysis software and ab-initio calculations this gives detailed insights into the studied materials.

MM 34.3 Wed 10:45 C 230

The Defect Distribution in the Near-Surface Region in Al alloys Studied by Positron Annihilation Spectroscopy — •Lucian Mathes[1], Vassily Vadimovitch Burwitz[1], Adrian Langrehr[1], Christoph Springl[1], Bastian Veltel[1], Emma Huntley[3], Andreas Wagner[2], Maik Butterling[2], Eric Hirschmann[2], Maciej Oskar Liedke[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TU München — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics — [3]Durham University

We have examined defects in pure and technical Al alloys on the atomic level using Positron Annihilation Spectroscopy. The influence of polishing (down to 40 nm OP-S) and heat treatment (T4 and T6) is explored in the near-surface region up to 6 μm in depth. We have determined the vacancy distribution by means of depth-resolved Doppler-broadening spectroscopy (DBS) using the slow positron beam at TUM. Further, we have characterized the defect type by depth-resolved Positron Annihilation Lifetime Spectroscopy (PALS) performed at the pulsed slow positron facility MePS at pELBE (HZDR).

MM 34.4 Wed 11:00 C 230

Structural Characterisation of Nanoporous Copper — •Prabhu Prasad Biswal[1], Samuel Graf[2], Marlene Eichlseder[3], Fernando Gustavo Warchomicka[3], Fabio Blaschke[4], Maximilian Fuchs[1], Eduardo Machado Charry[1], Alexander Bottaro[1], Karin Zojer[1], Roland Resel[1], and Eva-Maria Steyskal[2] — [1]Institute of Solid State Physics, Graz University of Technology — [2]Institute of Materials Physics, Graz University of Technology — [3]Institute of Materials Science, Joining and Forming, Graz University of Technology — [4]Institute of Chemical Engineering and Environmental Technology, Graz University of Technology

Nanoporous metals are metals with features in the pore structure in the range of 100 nm or less. Nanoporous copper (np-Cu) has recently attracted attention as an alternative to nanoporous gold or platinum. Our np-Cu is prepared by in-situ alloying of aluminium and copper using a 3D laser printer, followed by annealing at 530° C, and a subsequent de-alloying process to remove aluminium. The structural properties of the prepared Al-Cu alloy and np-Cu, including morphology, crystal structures, and chemical composition were systematically compared using X-ray diffraction and X-ray fluorescence spectroscopy; scanning electron microscopy provides surface topography and composition. In addition, the pore size distribution and internal surface area of np-Cu are quantified using micro-computed tomography and mercury intrusion porosimetry. After de-alloying, domains retain their spatial position and extension while their composition changes.

MM 34.5 Wed 11:15 C 230

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

Due to their excellent strength-to-weight ratio, heat-treatable Al-Cu alloys have been widely used since their invention. Although the hardening precipitates in these alloys are well-known, the early stages of formation and decomposition are still topic of ongoing research. Based on state-of-the-art scanning transmission electron microscopy, single Cu atoms can be imaged and natural ageing in form of Guinier*Preston zone formation accelerated by excess vacancies can be investigated. Scanning transmission electron microscopy is used to investigate the influence of different parameters, such as thermal history and the addition of trace elements, on early-stage precipitation in Al. In addition, resistivity, DSC and hardness measurements are performed to evaluate the temper state of the specimens. A better understanding of the mechanisms of precipitate formation and precipitate growth in these alloys could make it possible to further fine-tune material properties.

MM 35: Topical Session: Hydrogen in Materials: from Storage to Embrittlement VI

Time: Wednesday 11:45–13:00 Location: C 130

Topical Talk MM 35.1 Wed 11:45 C 130

Palladium nanoparticles as hydrogenation catalysts — •Petra de Jongh, Jessi van der Hoeven, and Oscar Brandt Corstius — Debye Institute for Nanomaterials Science, Utrecht University, Utrecht The Netherlands

Regarding metal hydrogen interaction, palladium is one of the most investigated systems. An interesting application of this interaction is the use of palladium as hydrogenation catalyst. Due to its electronic properties and hence strong interaction with the dihydrogen molecule, palladium is one of the fastest hydrogenation catalysts (about six orders of magnitude faster than for instance copper), but a challenge is to control the surface properties of palladium to such an extent that it is also selective.

In this contribution I will introduce supported Pd nanoparticles as hydrogenation catalysts, and share some recent results of our group on the effect of Pd nanoparticles size, and the influence of alloying these nanoparticles with a second metal such as copper or gold.

MM 35.2 Wed 12:15 C 130

In-situ TEM reduction of a solid oxide cell with NiO/YSZ and NiO/BZCY materials for fuel electrode — •Svetlana Korneychuk[1,2], Cedric Grosselindemann[1], Norbert H Menzler[3], André Weber[1], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]KNMFi, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Forschungszentrum Jülich GmbH, Jülich, Germany

Solid oxide fuel cells play a key role in the transition to the green economy. The quality of the electrode plays a major role in the performance and durability of a fuel cell. Ni/YSZ or Ni/BZCY fuel cell electrodes of solid oxide cells are commonly reduced from NiO/YSZ or NiO/BZCY under hydrogen atmosphere at high temperatures, prior to operation. The reduction results in a significant change in microstructure. As specific microstructural properties are crucial to achieve high performance and durability of the cell, a comprehensive understanding of the reduction process is required. Using in-situ TEM atmosphere system from Protochips we studied the electrode reduction at the H2 pressures up to 1 atmosphere and temperatures up to 850 °C [1] which fit the real working condition of a solid oxide cell. Grain boundaries and triple junctions between NiO and YSZ or BZCY are determined as the starting points of the reduction process at lower temperatures. The initial temperature of the reduction is crucial to achieve a high number of electrochemically active triple phase boundaries between Ni/YSZ and gas. [1] Korneychuk, S. et al., Rochester, NY October 17, 2023. https://doi.org/10.2139/ssrn.4604921

MM 35.3 Wed 12:30 C 130

Computational optimization of nanoalloy hydrogen sensors via composition and geometry — •Pernilla Ekborg-Tanner[1], Magnus Rahm[1], Victor Rosendal[1], Tuomas Rossi[2,1], Tomasz Antosiewicz[3,1], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Applied Physics, Aalto University, Aalto, Finland — [3]Faculty of Physics, University of Warsaw, Warsaw, Poland

Plasmonic hydrogen sensing based on nanoalloys could be a solution to the safety issues related to operating hydrogen gas under ambient conditions, which are currently hindering the hydrogen economy. In particular, random arrays of Pd-Au nanodisks have shown great potential as hysteresis-free, reliable hydrogen sensors. While several experimental studies have been conducted, computational studies necessary to efficiently span the rich parameter space in terms of nanodisk geometry and alloy composition are rare. Here, we therefore present a multi-scale modeling approach to hydrogen sensing from atomic scale ab-initio calculations (DFT, TD-DFT) to continuum scale electrodynamic simulations (FDTD) with the purpose of optimizing the sensitivity. In this work, the sensitivity is defined as the shift in peak position with respect to the absorbed hydrogen concentration. The sensitivity is highly tunable via the disk diameter. In addition, it displays a distinct two-regime behavior governed by peak splitting, in contrast to experimental studies. The peak splitting is, in turn, caused by an avoided crossing between the plasmon peak and an interband transition which comes into play at high H content.

MM 35.4 Wed 12:45 C 130

Probing hydrogen with high spatial resolution: a new correlative deformation/hydrogen sensing technique for hydrogen embrittlement study — •Maria Vrellou[1], Xufei Fang[1], Hans-Christian Schneider[1], Alexander Welle[2], Astrid Pundt[1], and Christoph Kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Karlsruhe, Germany

Hydrogen is one of the most promising alternatives to fossil fuels. The green hydrogen produced using energy from processes with low gas emissions or from renewable sources is considered as a potential game changer. However, hydrogen embrittlement (HE) is a major concern in hydrogen storage and transportation, and the underlying mechanisms need to be better addressed. Here, we present a novel approach aiming to isolate, observe and quantify the debated mechanisms responsible for HE. Our project, TRITIum based microMEchanics (TRITIME), aims to use techniques capable of achieving hydrogen imaging at quasi-atomistic resolution. APT and ToF-SIMS will be used to study the local and global tritium content in different microstructures in Ti and Zr samples that are susceptible to hydride formation, which is expected to provide better localization of the "hydrogen reservoir" facilitating hydrogen detection and quantification when employing the high-spatial-resolution techniques. To decipher the contribution of each one of the HE mechanisms, mechanical testing such as micro-pillar compression will be applied and studied.

MM 36: Liquid and Amorphous Materials I

Time: Wednesday 11:45–13:00 Location: C 243

MM 36.1 Wed 11:45 C 243

Influence of SRO and MRO on the plastic deformation behavior of amorphous metals — •Valeria Lemkova[1,2], Florian Spath[1], Pia Weihing[1], Tobias Thielen[1], Christian Motz[1], Florian Schäfer[1], and Ralf Busch[2] — [1]Materials Science and Methods, Saarland University Campus D2 3, 66123 Saarbruecken, Germany — [2]Metallic Materials, Saarland University Campus C6 4, 66123 Saarbruecken, Germany

The plastic deformation behavior of amorphous metals is not yet fully understood. In particular, shear transformation zones (STZ) are at the center of the discussion. In order to better understand and characterize them, nanoindentation was used to determine the so-called pop-in behavior as well as the strain rate sensitivity (SRS). The SRS provides information on the interaction of the STZ and shear band formation, while the pop-ins are directly related to STZ formation, i.e., the plastic deformation behavior. Strain rate tests were carried out on different amorphous metals, in particular Zr-based (ZrCuNiAlTi) and Ti-based (TiZrCuSAl), with different short range (SRO) and medium range order (MRO) determined via scattering experiments. In the results the correlation between SRO / MRO and the plastic deformation behavior is evaluated and discussed.

MM 36.2 Wed 12:00 C 243

crack-healing mechanisms in high entropy alloys under ion irradiation — •qi xu, daniel sopu, and jürgen eckert — Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, Leoben A-8700, Austria

High entropy alloys (HEAs) are potential candidate for advanced nuclear structural materials due to the outstanding mechanical properties and irradiation resistance in extreme conditions. However, microcracks, a common material damage, are introduced during the preparation and service processes, resulting in weakened structural integrity and irradiation resistance. In this work, an atomistic investigation of crack healing mechanisms in FeCoCrNiAl0.5 HEA under ion irradiation is provided by molecular dynamics (MD) simulations. Quantitative analysis of the point defect generation and recombination during the process of overlapping collision cascades are implemented to assess the irradiation response of cracked HEA. The interstitial defects generated in the core of the cascade during the first collision event diffuse to the crack surface, resulting in crack-healing during subsequent recrystallization. Additionally, the corresponding vacancies precipitate and form large-size vacancy clusters that generate stacking faults and complex dislocation networks distributed around the position of the healed crack. With increasing the number of overlapping cascades, the defects recombination rate increases and the phase stability is further improved. The crack healing engineering in HEA under ion irradiation could pave the way towards designing advanced nuclear materials.

MM 36.3 Wed 12:15 C 243

Influence of structural relaxation and composition on corrosion properties of Zr-based bulk metallic glass formers — •Benedikt Schmidt[1], Maximilian Frey[1], Florian Schäfer[2], Christian Motz[2], and Ralf Busch[1] — [1]Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany — [2]Chair of Materials Science and Methods, Saarland University, Campus D2.3, 66123 Saarbrücken, Germany

Bulk metallic glasses (BMGs) exhibit remarkable properties compared to crystalline alloys. They can surpass the strength of steels while also offering processability similar to polymers. Due to their amorphous structure and the resulting lack of grain boundaries, extensive attention has been directed toward the corrosion properties of these alloy systems. While previous studies have predominately focused on the comparison of the crystalline and amorphous state, the influence of structural relaxation of the glass remains poorly investigated. Through systematic sub-Tg annealing of a Zr-based BMG, we create samples with different fictive temperatures. Electrochemical analysis is performed via potentiodynamic polarization using a sodium chloride solution. We observe a consistent stability in the pitting potential, coupled with a shift of the free corrosion potential towards a more noble direction. Regarding a broader field of Zr-based systems, their corrosion mechanism is found to be mainly governed by selective corrosion as in case of the dezincification of brass. Notably, nickel emerges as a significantly influencing element in corrosion inhibition within these systems.

MM 36.4 Wed 12:30 C 243

Ni-Nb-P-based bulk glass-forming alloys: Superior material properties combined in one alloy family — •Lucas Ruschel and Ralf Busch — Chair of Metallic Materials, Saarland University, Saarbrücken 66123, Germany

Ni-Nb-based bulk glass-forming alloys are among the most promising amorphous metals for industrial applications due to their incomparable combination of strength, hardness, elasticity and plasticity. However, the main drawback is the limited glass-forming ability (GFA), narrowing the field of application to solely small components. A successful approach in alloy development is so-called minor alloying, where metallic glasses with improved properties and enhanced GFA are produced, if the proper minor alloying element is chosen for the respective base alloy. Here, minor additions of P to the binary Ni-Nb system increase the GFA up to 4 mm across a broad bulk glass forming region, culminating in a record value of 5 mm, which surpasses the binary $Ni_{62}Nb_{38}$ alloy by 150 %. Moreover, the primary precipitating phase, playing a crucial role for glass formation, is determined by container-less electrostatic levitation in-situ high-energy X-ray diffraction experiments. The mechanical properties of the new alloys are characterized in uniaxial compression tests and Vickers hardness measurements, showing a high engineering yield strength of 3 GPa, an extended plastic regime up to 10 % strain to failure and an increase of the hardness to a maximum value of 1000 HV5. Additionally, calorimetric measurements reveal an extended supercooled liquid region up to 69 K, permitting thermoplastic forming of amorphous feedstock material.

MM 36.5 Wed 12:45 C 243

Thermoplastic-patterned Ni-free Ti-based bulk metallic glass for biomedical research and its processing tolerance — Fei-Fan Cai[1,2], Andreu Blanquer[3], Miguel Brito Costa[4], Lukas Schweiger[1], Baran Sarac[2], A. Lindsay Greer[4], Jan Schroers[5], Christian Teichert[1], Carme Nogues[3], •Florian Spieckermann[1], and Jürgen Eckert[1,2] — [1]Montanuniversität Leoben, Austria — [2]Austrian Academy of Sciences, Austria — [3]Universitat Autonoma de Barcelona, Spain — [4]University of Cambridge, UK — [5]Yale University, USA

The advantageous mechanical properties and exceptional biocompatibility of Ni-free Ti-based bulk metallic glasses (BMGs) make them promising materials for biomedical applications. The glassy nature of BMGs allows them to be shaped and patterned via thermoplastic forming (TPF). The first part of this talk demonstrates the versatility of the TPF technique on Ti40Zr10Cu34Pd14Sn2 BMGs to create highly ordered patterns in micro- and nano-scales and a hierarchical structure integrating both patterns on one surface. The hierarchical structure fabricated by a two-step TPF process integrates 400 nm diameter hexagonal close-packed protrusions on 2.5 *2.5 μm^2 square protuberances and retains the beneficial mechanical properties of the as-cast materials. The second part of this talk focuses on the biocompatibility of Ti40Zr10Cu34Pd14Sn2 BMGs with four surface topographies (flat, micro-patterned, nano-patterned, and hierarchical-structured surfaces) using Saos-2 cell lines.

MM 37: Transport in Materials: Diffusion, Conduction of Charge or Heat IV

Time: Wednesday 11:45–12:45 Location: C 264

MM 37.1 Wed 11:45 C 264

Atomistic modelling of bulk and grain boundary diffusion for solid electrolyte Li$_6$PS$_5$Cl — ●Yongliang Ou[1], Yuji Ikeda[1], Sergiy Divinski[2], and Blazej Grabowski[1] — [1]Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Li$_6$PS$_5$Cl is a promising candidate for the solid electrolyte in all-solid-state Li-ion batteries. In applications, this material exits in a polycrystalline state with many grain boundaries (GBs) rather than a single-crystalline state. Atomistic modeling of Li$_6$PS$_5$Cl with GBs, however, remains rare due to high computational cost. Here, machine-learning interatomic potentials, specifically moment tensor potentials (MTPs), are employed to accelerate simulations while preserving the *ab initio* accuracy. Two tilt GBs $\Sigma3(1\bar{1}2)[110]$, $\Sigma3(\bar{1}11)[110]$ and one twist GB $\Sigma5(001)[001]$ are investigated, all of which exhibit low GB energies based on the annealing and quenching relaxation approach. Diffusion coefficients are calculated through mean square displacements obtained by molecular dynamics simulations. Enhanced Li diffusion compared to the perfect bulk is observed at GBs. A connection between GB morphology and its effects on Li diffusion is revealed, paving the way for improved solid electrolyte design through GB engineering.

MM 37.2 Wed 12:00 C 264

Navigating the Interface: Exploring Grain Boundaries in Solid-State Electrolytes through Ultrafast Interpretable ML Potentials — ●Tabea Huss, Carsten G. Staacke, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

The lithium thiophosphate (LPS) material class provides promising candidates for solid-state electrolytes (SSE) in lithium ion batteries due to high lithium ion conductivities and low material cost. 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 material performance and cycle stability.

Atomistic simulations are challenged by the complexity of these grain boundaries, having to both capture the complex chemistry of these materials and their low degree of order. Here, we tackle this with newly introduced ultra-fast interpretable machine learning potentials (UFP)[1] to combine the high accuracy of machine learned potentials with the speed of classical ones. This enables us to explore polycrystalline solid-solid interfaces within the LPS system on a grand scale, encompassing system sizes exceeding 10,000 atoms and time scales spanning multiple nanoseconds across substantial ensemble sizes. Ultimately we conduct a comprehensive analysis of grain boundaries in LPS aiming to understand their stability and their influence on the transport of lithium ions.

[1] S. R. Xie et al., npj Comp. Mater. 9, 162 (2023).

MM 37.3 Wed 12:15 C 264

Grain boundary diffusion of 57Co in Cu SIGMA-5 (310) bicrystals — ●Esakkiraja Neelamegan[1], Daniel Gaertner[1], Hui Ding[2], Anoosheh Akbari[1], Christian H Liebscher[2], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, 48149 Germany — [2]Structure and Nano- / Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Diffusion of 57Co in pure copper SIGMA-5(310)[001] bicrystals is investigated using the radiotracer technique. The measurements are performed both in type B ($>$ 950 K) and type C ($<$ 850 K) kinetics regimes after Harrison classification. The tracer diffusion experiments are conducted by varying the amount of the applied 57Co tracer solution, and the characteristic changes in the shape of the penetration profiles are related to the Co segregation-induced changes of the grain boundary structure.

MM 37.4 Wed 12:30 C 264

Grain- and phase boundary diffusion in AlCoCrFeNi2.1 compositionally complex alloy — ●Heng Zhang, Mohan Muralikrishna, Sergiy Divinski, and Gehard Wilde — Institute of Materials Physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149, Muenster

Grain and phase boundary diffusion of 63Ni is investigated in a Al-Co-Cr-Fe-Ni multi-principal element system. For better understanding on the influence of chemical complexity and the crystal structure on the atomic transport, Ni diffusion is systematically measured in two-phase (FCC+B2) eutectic AlCoCrFeNi2.1 alloy and its single phase FCC and B2 counterparts. Grain boundary (GB) diffusion of Ni is found to be similar in all three alloys substantiating enhanced phase boundary diffusion in the eutectic alloy on par with GB diffusion in single phase alloys. However, when compared on the homologous scale, GB diffusion in FCC and eutectic alloys is found to be similar and it is faster in the single phase B2 HEA. The measured GB diffusivities are compared with the GB self-diffusion rates in pure elements and alloys. An impact of chemical complexity on grain and phase boundary diffusion is discussed in terms of the *sluggish* diffusion concept invented for the high-entropy alloys.

MM 38: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials III (joint session MM/KFM)

Time: Wednesday 11:45–13:00 Location: C 230

MM 38.1 Wed 11:45 C 230

Atomic cluster expansion for binary Ag-Pd alloys — Yanyan Liang, ●Matous Mrovec, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

Binary alloys of silver and palladium have recently attracted increased attention due to their applications 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 as well as large scale simulations of mechanical properties. In this work, we present an atomic cluster expansion (ACE) parameterized for Ag-Pd with ab-initio accuracy. We show that the ACE parametrization provides an accurate description of the elastic, structural and thermodynamic properties of both elements as well as their compounds. We demonstrate the computational efficiency and the applicability of the developed potential for atomistic simulations of complex phenomena in elemental as well as Ag-Pd systems.

MM 38.2 Wed 12:00 C 230

Training strategies for machine-learning potentials suitable to simulate mechanical response of ceramics — ●Shuyao Lin[1,2], Zhuo Chen[3], Luis Casillas-Trujillo[2], Ferenc Tasnadi[2], Zaoli Zhang[3], Lars Hultman[2], Paul H. Mayrhofer[1], Davide G. Sangiovanni[2], and Nikola Koutna[1,2] — [1]Institute of Materials Science and Technology, TU Wien, A-1060, Vienna, Austria — [2]Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-58183, Linköping, Sweden — [3]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, A-8700, Leoben, Austria

Machine-learning interatomic potentials (MLIPs) offer a powerful avenue for simulations beyond length and timescales of *ab initio* methods. In particular, MLIPs enable investigations of mechanical properties and fracture behaviour of materials with supercell sizes, loading geometries and temperatures relevant for real operation conditions. Using the example of hard TiB$_2$ ceramic, in this talk we propose a strategy for fitting MLIPs suitable to simulate mechanical response of monocrystals from atomic to nanoscale, including strains until fracture and deformation-induced phase transformations. After validation, the best-performing MLIP is employed to carry out molecular dynamics simulations of various loading conditions, with main focus on tensile and shear deformation. Consequently, we derive size-dependent trends in theoretical strength, toughness, and crack initiation patterns of TiB_2. To approach experimental observations, we additionally apply our MLIP to models containing a pre-crack and/or grain boundaries.

MM 38.3 Wed 12:15 C 230

Investigating the yield stress anomaly of Ni_3Al with physically informed machine-learning potential — •Xiang Xu, Xi Zhang, Siegfried Schmauder, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

The anomalously increasing yield stress with temperature of some intermetallics is predominately controlled by the Kear-Wilsdorf lock (KWL), of which the formation and unlocking are closely related to a cross-slip process. Yet so far, knowledge of this cross-lip process is limited, leading to significant approximations in existing models for predicting the mechanical behavior of those materials. In this study, molecular dynamics simulations were conducted by using a physically informed machine-learning potential to replicate dislocation activities of Ni_3Al. For the first time, it is observed that the formation and unlocking of KWL occurs with a step-by-step cross-slip process, of which the distance varies between one or two atomic planes inside each step. Moreover, a strong temperature dependence of the necessary stress to unlock a KWL was discovered, differing from previous approximations. This study not only advances the understanding on the yield stress anomaly in Ni_3Al, and also establishes a systematic workflow for yielding multiscale atomistic simulations using machine-learning potentials.

MM 38.4 Wed 12:30 C 230

The Effect of Al Sublattice in Tuning Elastic Anisotropy in Fe-Ta-Al Laves Phases — •Nisa Ulumuddin, Christina Gasper, Zhuocheng Xie, and Sandra Korte-Kerzel — RWTH Aachen Institut für Metallkunde und Materialphysik

As Laves phases found in alloys are often undesirable due to its brittleness, fundamental knowledge on tuning its mechanical properties can pave the pathway for the enhanced design of engineering alloys. The structural motifs arising from the substitutional mixing of Al into the Fe_2Ta Laves phase at varying Al:Fe ratios were studied by first-principles. The presence of an Al sublattice was found to reduce elastic anisotropy, owing to changes within the bonding nature of the crystal. They induce a higher degree of metallic bonding within the crystal as Al is relatively less electronegative than Fe. The increased degree of non-directional bonding decreases the directional preference for elastic deformation. These results signify the possibility of adjusting the mechanical properties of intermetallics by considering the electronic properties of their individual components.

MM 38.5 Wed 12:45 C 230

Effect of the V-VIB groups ternary elements on the properties of Ti2AlM-type O-phases: A first-principles study — •Zeinab Heidari Pebdani[1,2], Florian Pyczak[1,2], and Rebecca Janisch[3] — [1]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]BTU Cottbus-Senftenberg, Cottbus, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Despite the recent introduction of γ-TiAl-based alloys into service, the assessment of TiAl-alloys based on the ternary Ti2AlM orthorhombic O-phase, which are promising high-temperature structural materials, has not yet been completed. The focus of this contribution is on the impact of ternary alloying elements of the V-VIB groups of the periodic table on phase stability, structural, mechanical, thermal properties, and lattice dynamics of Ti2AlM (M= V, Nb, Ta, Mo, W) type O-phases. All Ti2AlM compounds satisfy the Born stability criteria, but their properties are largely affected by the ternary element M. According to the energy of formation, Ti2AlMo is the most stable type of O-phase. The bonding behavior of all compounds is investigated by analyzing the electronic density of state plots. It was found that stronger Ti-M bonding enhances while stronger Ti-Al bonding decreases the ductility in the Ti2AlM compounds. The thermodynamic stability of the intermetallic phases is key information to further develop these materials. To consider this we have used a set of comprehensive ab initio methods, in order to determine the temperature dependence of the properties of those intermetallic phases.

MM 39: Invited Talk: Yolita Eggeler

Time: Wednesday 15:00–15:30 Location: C 130

Invited Talk MM 39.1 Wed 15:00 C 130

Exploring Creep-Induced Planar Faults: Segregation Dynamics and Defect Phase Transformations in High Performance Alloys — •Yolita Eggeler — KIT - Laboratory for electron microscopy

This study investigates the extent of segregation to creep-induced planar faults in superalloy ERBO1 under 1% and 2% creep strains. Findings show that increasing creep strain leads to a rise in dislocation density, resulting in more planar faults. Notably, segregation levels in 1% and 2% strains are comparable, indicating saturation of the fault with relevant elements and the consistent establishment of a local defect phase equilibrium, irrespective of strain magnitude. Acknowledging this constancy, the study recognizes a critical time beyond which the hypothesis may no longer hold true, influenced by factors such as diffusion, solute element cloud, and temperature. Utilizing MEMS-based heating chips and efficient energy-dispersive X-ray spectroscopy detectors within the transmission electron microscope (TEM), enable to explore the kinetics of defect phase transformations through local segregation during isothermal exposure on the nanometer scale. With a nano-diffusion-couple (NDC) approach demonstrated at the interfaces of a two-phase model system, the NDC approach is extended to study segregation phenomena at planar defects. Chemical segregation near planar defects indicates an apparent defect phase transformation within the parent phase, influencing the high-temperature properties of the alloy.

MM 40: Focus Session: Battery Materials – Experimental Characterisation and Safety Testing (joint session KFM/MM)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques , thermal characterisation techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Chair: Carlos Ziebert (KIT Karlsruhe)

Time: Wednesday 15:00–19:05 Location: EMH 225

Invited Talk MM 40.1 Wed 15:00 EMH 225

Reversible and irreversible heat effects in batteries and battery materials — •Andreas Jossen — Technical University of Munich, School of Engineering and Design, Department of Energy and Process Engineering, Chair for Electrical Energy Storage Technology, Arcisstrasse 21, 80333 Munich, Germany

Heat generation within batteries is caused by different effects, as entropy, over-potentials and voltage hysteresis. These effects depend on the state of charge and the state of health of the battery and the resulting temperature strongly influences the performance of the system. Therefore measuring of these heat effects is of high interest to support the material and cell design development. Especially of large format cells, as used in electric vehicles, the heat balance strongly influences the fast charge capability on system level. The presentation introduces the different effects and describes measurement methods (calorimetric and electrical based) and discusses the challenges for the different methods. Improved measurement methods are presented and measurement examples for some high-energy materials are discussed. An example where upscaling from a material level to large format cell is shown

MM 40.2 Wed 15:30 EMH 225

Temperature dependency of the heat capacity of Lithium-ion batteries during Heat-Wait-Seek Tests in Accelerating Rate Calorimetry — •Philipp Finster, Hans J. Seifert, and Carlos Ziebert — Karlsruhe Institute of Technology (KIT), Institute of Applied Materials - Applied Materials Physics (IAM-AWP), Eggenstein-Leopoldshafen, Germany)

The Heat-Wait-Seek test in Accelerating Rate Calorimeter (ARC) can be used to estimate the safety performance of Lithium-ion cells by extracting parameters such as critical temperatures or generated heat. To calculate the generated heat, it is essential to know the heat capacity of the cell as a function of temperature.

In this study we show an accurate way to calculate the heat capacity of the cell, based on its individual components with respect to temperature. Additionally, we will discuss time dependency of the heat capacity, for instance while melting of the separator or venting. Using this dependence of temperature results in a significant difference in the calculated heat capacity of about 15 % in the temperature range from 298 K to 498 K. In this work the approach is applied to commercial type 21700 cells. The cells were measured in an ES-ARC from Thermal Hazard Technology, UK. The generated heat was compared for either fresh cells or cells after cyclic aging.

With this approach the generated heat in abuse tests can be predicted more accurately to simulate the propagation of heat during a single cell failure in a pack or to calculate the appropriate thickness of a heat barrier for safer battery packs.

MM 40.3 Wed 15:50 EMH 225

Thermal Runaway analysis of lithium-ion batteries with different electrolyte compositions — •Karsten Geuder, Hans Jürgen Seifert, and Carlos Ziebert — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Investigation of the safety of lithium-ion batteries, particularly with respect to thermal runaway, is critical because of the wide application of these batteries. This study specifically examines the influence of electrolyte and additives on battery safety and aims to improve our understanding of thermal runaway in full cells through comparative analysis.

Unlike commercial lithium-ion batteries, the electrolyte composition is well known. The control electrolyte of the 1Ah pouch cells is a 3:7 mixture of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). In addition, we used the control electrolyte with either 5% vinylene carbonate (VC) or 5% fluoroethylene carbonate (FEC). To assign the different thermal processes and reactions in the full cells, the dry cells were disassembled and the components were analyzed by differential scanning calorimetry. The full cells were characterized for their thermal runaway behavior using both Heat-Wait-Seek and overcharge tests in accelerating rate calorimeters. We were able to correlate the endothermic behavior of the full cell at about 115 °C with the onset of separator melting. A comprehensive understanding of thermal runaway is critical to ensuring the safety of lithium-ion batteries. An accurate understanding of the electrolyte composition provides deeper insight into its safety implications.

MM 40.4 Wed 16:10 EMH 225

Comparison of thermal safety of new and aged commercial 21700 lithium-ion batteries with different cathode materials by Accelerating Rate Calorimetry (ARC) — •Sebastian Ohneseit, Nils Uhlmann, Hans Jürgen Seifert, and Carlos Ziebert — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Applied Materials Physics (IAM-AWP), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Cylindrical lithium-ion batteries (LIB) of type 21700 have multifaceted usage applications, such as consumer goods, battery electric and hybrid electric vehicles. In consequence, their safety in new and aged state is of particular interest. In this experimental study, the different cathode materials NMC, NCA and LFP were compared, as well as high power and high energy cells. Calendar and cyclic aging with different test conditions (temperature, discharge rate) was performed on the listed cell types and subsequently safety tests were performed on the aged cells, in comparison to results of new cells of the same type. Thermal abuse was done by the heat-wait-seek test in an Accelerating Rate Calorimeter (ARC). Several critical temperatures and temperature rates, as well as exothermal data, were determined. Furthermore, the grade of destruction and mass loss was determined, and all data was compared for aged and unaged cells. It was found that, for aged NMC and NCA cells, the aging parameter modified the exothermal reaction onset and overall, a lower maximum temperature was found for the aged cell state. LFP cells reacted, as expected, at significantly higher temperatures, making the cell chemistry considerably safer.

MM 40.5 Wed 16:30 EMH 225

Are Li-ion cells safe for 2nd-Life Applications - The Case of Lithium Plating — •Thomas Waldmann[1,2], Gabriela G. Gerosa[1], Max Feinauer[1], Markus Hölzle[1], and Margret Wohlfahrt-Mehrens[1,2] — [1]Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW), Helmholtzstrasse 8, D-89081 Ulm — [2]Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Helmholtzstrasse 11, D-89081 Ulm

Increased sustainability and reduced dependence on foreign critical resources (e.g. Co, Ni, Li) go hand in hand with increased cycle life and re-use of aged Li-ion batteries in 2nd-life applications before recycling. However, there is a lack of knowledge on the safety of aged cells with the mechanism of lithium plating. Lithium plating leads to fast aging of Li-ion cells due to reaction of the deposited lithium with electrolyte and formation of ”dead lithium”. We show results on the influence of lithium plating in commercial Li-ion cells in the 1st-life on safety in 2nd-life. Possibilities to detect and avoid lithium plating which we investigated recently are discussed. Arrhenius plots of the aging rate in the 1st-life show the typical V-shape and the transition to lithium plating as main aging mechanism below 25°C. Our safety tests show higher hazard levels for cells with lithium plating after the 1st-life. Therefore, lithium plating is an aging mechanism which is to be avoided. Possibilities are shown to avoid Li plating and for early detection of unsafe behavior.

15 min. break

MM 40.6 Wed 17:05 EMH 225

Microstructural Impact on Filament Growth in All Solid-state Sodium Batteries — •Ziming Ding[1], Yush Tang[1], Till Ortmann[2], Janis Kevin Eckhardt[2], Marcus Rohnke[2], Georgian Melinte[1], Christian Heiliger[2], Jürgen Janek[1,2], and Christian Kübel[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Institute for Physical Chemistry and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany — [3]Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Although the intergranular growth mechanism in inorganic solid electrolytes (SEs) based lithium-based all solid-state batteries (ASSBs) is well studied, there is still much to be learned for sodium-based ASSBs. The polycrystalline Na-β"-alumina is selected as a model material to investigate its microstructural impact on Na-filament growth. Using in situ biasing transmission electron microscopy, the Na-filament growth at the interface between the SE and electrode and grain boundaries (GBs) within the SE, were observed during Na deposition. The relationship between the microstructure of SE and filaments is further studied through the orientation analysis and corelative imaging. It is found that anisotropic ion transport due to layered crystal structure can contribute to distinctive Na-ion transport behaviors at different GBs during operation and influence the Na-filament growth. This work helps to understand Na-filament formation and how a critical filament network might form leading to failure of the battery.

MM 40.7 Wed 17:25 EMH 225

Computational and experimental investigation of Na and Y co-doping on electrochemical performance of LiNi0.8Co0.15Al0.05O2 cathode material for Li-ion batteries — Sahar Ziraki[1], •Mansour Kanani[1], Babak Hashemi[1], and Mohammad Mohsen Loghavi[2] — [1]Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran — [2]Department of Energy Storage, Institute of Mechanics, Shiraz, Ira

LiNi0.8Co0.15Al0.05O2 (NCA) has attracted a lot of attention owing to its high voltage, specific energy density, and specific capacity. However, the cycle durability of the NCA material is still a challenge. In this study, the addition of sodium (Na) on Li-site and yttrium (Y) on metal-site, and their co-doping into NCA material, were investigated experimentally and theoretically. For the first time, we proposed a framework for parameterization of the structural and thermal stability of NCA during the lithiation/delithiation process in terms of first-principle density functional theory (DFT) calculations. The computational results confirmed the positive effect of Na+ and Y3+ on the structural and thermal stability of the NCA cathode systematically. Following those outcomes, different percentages of the dopants were added to the cathode material experimentally, and electrochemical tests were performed. The underlying mechanisms of observed experimental improvements were interpreted and discussed according to the computational outcomes.

MM 40.8 Wed 17:45 EMH 225

Pits and Traps in the Impedance Analysis of Ionic Conductors — •Janis K. Eckhardt[1,2,3], Sascha Kremer[2,3], Matthias T. Elm[2,3,4], Peter J. Klar[3,4], Jürgen Janek[2,3], and Christian Heiliger[1,3] — [1]Institute for Theoretical Physics, Justus Liebig University, Giessen D-35392, Germany — [2]Institute of Physical Chemistry, Justus Liebig University, Giessen D-35392, Germany — [3]Center for Materials Research (ZfM), Justus Liebig University, Giessen D-35392, Germany — [4]Institute of Experimental Physics I, Justus Liebig University, Giessen D-35392, Germany

The development of innovative electrochemical storage systems, such as solid-state batteries, is critical for achieving climate neutrality and sustainability goals. Several hurdles must be overcome before such technologies are ready for the market. Impedance spectroscopy is a powerful method for characterizing the electrical transport properties of new materials and for monitoring systems in operation. Although it is an older measurement technique, the interpretation of data for inhomogeneous solid-state systems lacks established concepts for reliable results. Thus, we use 3D electrical network models for spatially-resolved transport simulations and systematic investigation of the influence of sample microstructure and solid-solid interface morphology. The material-specific transport quantities derived from 1D models (e.g., brick layer model) sometimes exhibit inaccuracies of several orders of magnitude. In addition, the impedance response of the system exhibits geometric signatures that cannot be adequately represented in 1D physically motivated circuit models, e.g., current constriction.

MM 40.9 Wed 18:05 EMH 225

Vacancies on the Lithium-Sublattice in the Solid-State Electrolyte LLZO employing Positron Annihilation Spectroscopy — Dominik Boras[1], Andreas Kohrmann[1], Daniel Wagner[1], Daniel Göbel[1], Janez Kosir[2], Tanja Kallio[2], and •Torsten E.M. Staab[1] — [1]Institute for Functional Materials and Biofabrication, Julius-Maximilians Universität Würzburg, D-97070 Würzburg, Röntgenring 11 — [2]Department of Chemistry, Aalto University, Kemistintie 1, FIN-02015 Espoo

We characterise the electrolyte LLZO for all solid-state batteries. LLZO ($Li_7La_3Zr_2O_{12}$) samples have been synthesised via the mixed-oxide route, i.e. grinding and calcination, grinding again, then pressing and finally sintering the pellets. We varied the doping (Fe, Al) and the excess Li content. The formed phases (cubic and tetragonal) have been characterised by XRD, while the lattice defects have been investigated by the method of positron annihilation lifetime spectroscopy (PALS). By PALS we were able to see clear differences after calcination when varying the lithium excess. Measuring powder with increasing Li-excess a lifetime component, which could be related to the bulk crystal significantly decreases from 220ps to 190ps. This may be an indication of more and more filled Li-lattice site after the calcination step. Sintered pellets showed two different positron lifetimes (190 / 200ps and 326 / 374ps) for both un-doped / Al-doped samples. This first attempt shows the potential of PALS to characterise all sold-state electrolytes with respect to defects and the occupation of crystal lattice site influencing the mobility of Li ions.

MM 40.10 Wed 18:25 EMH 225

Exploring Polaron Stability and Defect Structures in $Li_4Ti_5O_{12}$ (LTO): A Combined Theoretical and Experimental Approach — •Yu-Te Chan[1], Matthias Kick[2], Cristina Grosu[2], Christoph Scheurer[1], and Harald Oberhofer[3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]University of Bayreuth

Spinel $Li_4Ti_5O_{12}$ (LTO) is a promising anode material for next-generation all-solid-state Li-ion batteries (ASSB) due to its "zero strain" charge/discharge behavior. Pristine, white LTO possesses poor ionic and electronic conductivity. Through tailoring the sintering protocol, one can produce oxygen vacancies accompanied by polaron formation, resulting in a performant, blue LTO material.

By performing Hubbard corrected density-functional theory (DFT+U) calculations we are able to show that polaron formation and a possible polaron hopping mechanism play a significant role in enhancing electronic conductivity and in boosting Li$^+$ diffusion, in line with the experimentally observed improved conductivities.[1] We pair these findings with positron lifetime spectroscopy (PALS) to study the charge carriers' (polaron and Li$^+$) behavior and the defect structures produced in the sintering. We developed a machine-learned potential to study the dynamics of the polaron and the structural defects measured from PALS, reaching a rather complete picture of the bulk vs. surface defect chemistry in LTO particles.

[1] M. Kick *et al.*, J. Phys. Chem. Lett. **11**, 2535 (2020); ACS Appl. Energy Mater. **4**, 8583 (2021).

MM 40.11 Wed 18:45 EMH 225

Partially substituted metal sulfide anodes for high-performance sodium-ion batteries — •Zidong Wang — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to sodium resources' abundance and easy availability, sodium-ion battery technology has attracted extensive research interest and made significant progress in recent years. Among the various anode materials used for sodium-ion battery anodes, transition metal sulfides, especially bimetallic sulfides, have great potential due to their high capacity and electrochemical activity. In this work, the original bimetallic sulfide cations were partially replaced to improve the performance further. In this strategy, the synergistic effect of multi-metal cations will result in superior energy absorption and enhancement. Metal elements with different oxidation states can produce higher capacity through synergistic effects with each other. Mn-Ni-Co-S with 10% substitution showed satisfactory capacity (721.09 mAh/g at 300 mA/g and 662.58 mAh/g after 20 cycles) and excellent cycle life (85.41% capacity retention after 1000 cycles at 2000 mA/g).

MM 41: Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides I (joint session DS/MM/O)

MXenes, two-dimensional transition metal carbides, nitrides and carbonitrides, constitute one of the most rapidly growing class of 2D materials. Discovered in 2010, they have demonstrated exceptional physical, chemical, and electronic properties leading to potential applications in various fields, such as energy storage, catalysis, electromagnetic interference shielding, sensing, and biomedicine. The fundamental physical properties of MXenes are governed by their chemical composition and great research efforts are currently devoted to expanding the range of existing MXenes by tuning their stoichiometry, morphology and surface chemistry as well as adding tailored defects that can bring new functionalities. In this Focus Session, new developments related to MXene synthesis and characterization will be presented. The fundamental physical properties and interfacial processes correlated with MXene surface chemistry, defects and interlayer confinement will be discussed.

Organizers:

Dr. Tristan Petit, Head of the Young Investigator Group Nanoscale Solid-Liquid Interfaces, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Prof. Vincent Mauchamp, Institut Pprime, CNRS-Université de Poitiers-ISAE ENSMA, Poitiers, France

Time: Wednesday 15:00–17:00 Location: A 053

Introduction Focus Session on MXene - V. Mauchamp & T. Petit

Invited Talk MM 41.1 Wed 15:15 A 053

Sustainable synthesis of MXenes and their precursors — •Jesus Gonzalez-Julian[1], Nima Amousa[1], and Filipa Oliveira[2] — [1]Chair of Ceramics, Institute of Mineral Engineering (GHI), RWTH Aachen University, 52074 Aachen, Germany — [2]Department of Inorganic Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic

Synthesis of MXenes is typically performed using HF - or forming in-situ HF through the reaction between LiF and HCl, but this chemical etching presents some limitations. HF is highly corrosive and toxic, requiring specific safety regulations, and the chemical etching is highly exothermic, limiting the amount of MXenes that can be produced in the range of grams. These two points are hindering the transfer of MXenes to real applications, despite the excellent properties of these 2D materials. Consequently, new synthesis processes are required to overcome these problems. In this work, we will present a novel sustainable synthesis route for the synthesis of the precursors (MAX phases) and the chemical etching, which is referenced as Molten Salt Shielded Synthesis or MS3. MS3 is carried out at lower temperatures than conventional synthesis routes, in air instead inert atmospheres, and does not require any milling step to obtain fine and loose powders.

MM 41.2 Wed 15:45 A 053

Tuning the molten salt etching process by in situ XRD — •Julian T. Müller, Aleksander Gurlo, and Maged F. Bekheet — Technische Universität Berlin, Faculty III Process Sciences, Institute of Material Science and Technology, Chair of Advanced Ceramic Materials, Straße des 17. Juni 135, 10623 Berlin, Germany

MXenes, whose properties are mainly defined by their chemical composition and surface terminations, could be synthesized by etching an A element (A = Al, Si, etc.) from the parent MAX phase using hydrofluoric acid. This acid is of high risk to human health and leads to fluorine terminations on the surface of MXene, which are difficult to alter and may be detrimental for certain applications, e.g. electrodes in different battery systems. Etching via molten salt formation offers an alternative, less harmful way. By sophisticated selection of salts, it is possible to adjust the surface terminations and pave the way for a new generation of tailored MXenes. Gaining insight into the molten salt etching process and tuning its process parameters such as temperature, duration, and precursor ratio are keys to ensuring a qualitative MXene and saving time, energy, and cost. To support this, we are currently establishing an in situ XRD setup at the Advanced Light Source of the Lawrence Berkeley National Laboratory. It will allow measurements under various gas atmospheres up to 1450 °C and 50 bars, including a vapour phase. In the first molten salt etching experiments, we successfully gained knowledge on the etching onset, duration, and phase composition. With this measurement setup, the synthesis of MAX phases and many MXene and salt combinations await to be explored.

MM 41.3 Wed 16:00 A 053

Preparation of Magnetic MXenes by Fe intercalation — Tim Salzmann[1], Hanna Pazniak[2], Thierry Ouisse[2], Fabrice Wilhelm[3], Andrei Rogalev[3], Ralf Meckenstock[1], Ivan Tarasov[1], Michael Farle[1], and •Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France — [3]European Synchrotron Radiation Facility, Grenoble, France

Yet, the success of generating magnetic MXenes remains very limited since Fe, Co or Ni are incompatible with MAX phase precursors. We present an alternative approach to master magnetic properties of 2D MXenes by intercalating Fe into $\mathrm{Ti_3C_2T_x}$ MXene thin films on $\mathrm{Si/SiO_2}$ in UHV conditions. Annealing of bare MXenes at T = 1023 K removes -F, -Cl and -OH. The intercalation of Fe is studied by depositing a 6 nm film on top of the MXenes and subsequent annealing. XRD shows an increase of the interplanar spacing between MXene sheets of 0.16 ± 0.02 nm. XPS and XANES reveal that Fe remains metallic and Fe diffuses 30 nm deep into the multilayers while MXenes keep intact. We study the magnetic properties by VSM and FMR. VSM suggests a new magnetic phase with $M_S = 660 \pm 80$ kA/m and a Curie temperature of 485 K while angular-dependent FMR at 9 GHz and 300 K shows two ferromagnetic and one paramagnetic signals, which we address to the remaining Fe on top and the intercalated Fe in form of quasi 2D disks and isolated Fe ions. Funded by DFG (530103526). Support by CRC/TRR 270 (405553726) is acknowledged.

MM 41.4 Wed 16:15 A 053

synthesis and characterization of 2D Mo/Ti solid solutions based MXene for hydrogen evolution reaction in alkaline media. — Lola Loupias[1], Claudia Morais[1], Sophie Morisset[1], Christine Canaff[1], Zheming Li[1], Patrick Chartier[2], Vincent Mauchamp[2], Thierry Cabioc'h[2], Aurélien Habrioux[1], and •Stéphane Célérier[1] — [1]Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP), Université de Poitiers, CNRS, F-86073 Poitiers, France — [2]Institut Pprime, UPR 3346 CNRS, Université de Poitiers, ISAE-ENSMA, BP 30179, 86962 Futuroscope-Chasseneuil Cedex, France

2D MXenes have gained an ever-increasing attention in various application fields. Their properties can be strongly tuned by modifying the M element in the Mn+1XnTx structure. Among them, Mo-based MXenes are beginning to be successfully explored in many areas. This work focuses on the synthesis and characterization of (Mo,Ti)n+1CnTx MXenes to understand their complex chemistry and to compare them with those of mono-metallic Mo2CTx and Ti3C2Tx. The potential of these materials as HER (hydrogen evolution reaction) catalysts is determined in alkaline medium. It is shown that Mo2Ti2C3Tx MXenes are a credible alternative to Mo2CTx MXenes since the surface properties of both MXenes are similar while their composition is quite different. Indeed, (Mo,Ti)n+1CnTx require lower temperatures and shorter time for the synthesis than for Mo2CTx, a great advantage from an industrial point of view. Finally, some avenues for improving the performance of MXenes for HER will also be described.

MM 41.5 Wed 16:30 A 053

MXenes as support for transition metal oxides electrocatalysts for water splitting application — •Axel Zuber[1], Zdeněk Sofer[2], and Michelle Browne[1] — [1]CE-NESD, Helmholtz Zentrum Berlin für Materialien und Energie, Berlin (Federal Republic of Germany) — [2]Department of Inorganic Chemistry, University of Chemistry and Technology, Prague (Czeck Republic)

To reduce the cost of energy conversion and tend towards a greener energy production, research has been trying to use first-row transition metal-based catalysts for water splitting. Despite their good activity for the oxygen evolution reaction, transition metal oxides (TMOs) performance is hindered by their low conductivity and instability under potential. To improve it, recent works have successfully combined them chemically with conductive 2D transition metal carbides and nitrides (MXenes). The rich chemistry, large surface area and conductivity of MXenes make them excellent candidates as electrocatalyst supports, but they are also keen to oxidize in water which induces a loss of these properties. In this study, different MXenes were combined with transition metal oxides and tested as electrodes for the oxygen evolution reaction. The stability of the MXene structure as well as the resulting compound performance for the oxygen evolution reaction were investigated. The electrode materials remained stable and allowed to improve the oxygen evolution reaction overpotential of the transition metal oxide.

MM 41.6 Wed 16:45 A 053

Infrared and Raman spectroscopic analysis of functionalized graphene and Mxene layers — •Karsten Hinrichs[1], Mailis Lounasvuori[2], Fatima Akhtar[2], Namrata Sharma[2], Tristan Petit[2], and Jörg Rappich[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Application Laboratories Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH 14109 Berlin, Germany

Functionalized 2D-conductive materials like graphene and Mxene layers are interesting templates for catalysis but are also important for building of optical and electro-chemical sensors. Spectroscopic Raman and infrared (IR) ellipsometry analysis can access complementary information on the conductive material but also the ultrathin functional organic layer, respectively. Thereby bands due to molecular vibrations and phonons as well as free carrier absorptions are related to chemical and structural material properties. We acknowledge financial support by the European Union through EFRE 1.8/13.

MM 42: Topical Session: In Situ and Multimodal Microscopy in Materials Physics I (joint session MM/KFM)

Time: Wednesday 15:30–18:00 Location: C 130

Topical Talk MM 42.1 Wed 15:30 C 130

Charges, Structure, Properties - Concepts and Applications of four-dimensional electron microscopy — •Knut Müller-Caspary[1,3], Benedikt Diederichs[1,2], Ziria Herdegen[1], Tizian Lorenzen[1], Felix Dushimineza[1,3], Max Leo Leidl[1,3], Achim Strauch[3], and Frank Filbir[2] — [1]Ludwig-Maximilians-Universität München, Dept. of Chemistry, Butenandtstr. 11, 81377 München — [2]Institute of Biological and Medical Imaging, Helmholtz Zentrum München, 85764 Neuherberg, Germany — [3]Forschungszentrum Jülich, Wilhelm Johnen Str., 52425 Jülich

Scanning an electron probe across a specimen and recording a diffraction pattern at each scan point established 4D-STEM as a versatile concept to characterise materials. We start with a very brief introduction of mapping electric fields and electrostatic potentials by using direct methods such as centre-of-mass imaging and analytical ptychographic solutions to the inverse single-scattering problem. Applications to large-scale electric field mapping and 2D materials will be shown. For thicker specimens, structure retrieval needs to invert multiple scattering. In this respect, we report a parametric inverse multislice concept in which both partial coherence of the probe and multiple frozen phonon states are taken into account. In particular, we investigate the impact of thermal diffuse scattering on different inverse multislice approaches. The concept is demonstrated via simulations first, and then applied to measure ionic displacements in ferroelectrics with picometre precision.

MM 42.2 Wed 16:00 C 130

TEM investigations of local structure and dynamics in PdNiP bulk metallic glass — •Olivia Vaerst[1], Martin Peterlechner[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Karlsruhe Institute of Technology, Laboratory for Electron Microscopy (LEM), Karlsruhe, Germany

The bulk metallic glass PdNiP is kinetically highly stable against crystallisation and therefore often used as a model system for investigations of the glassy state. Such investigations include experiments to further explore the glass formation and the structure-property relations of metallic glasses. In this work, the focus lies on understanding the atomic structure and local mobility of PdNiP in various thermo-mechanical states. For this purpose, multimodal transmission electron microscopy (TEM) measurements are performed using advanced techniques. The main method used is electron correlation microscopy (ECM), where diffracted intensities of a time series of dark-field images are correlated to deduce structural dynamics parameters with nanometer spatial resolution. A systematic analysis of the effect of varying electron beam parameters on the dynamics is conducted and optimal measuring parameters for PdNiP are determined. 4D-STEM fluctuation electron microscopy (FEM) is used for complementary structural investigations concerning the medium-range order of the different thermo-mechanical material states. The results on local dynamics and structural properties are discussed with respect to properties measured by macroscopically averaging methods.

MM 42.3 Wed 16:15 C 130

Strain mapping of a sigma 5(310) grain boundary in a Cu bi-crystal using scanning transmission electron microscopy — •Anoosheh Akbari[1], Harald Rösner[1], Esakkiraja Neelamegan[1], Hui Ding[2], Christian.H Liebscher[2], Sergiy Divinskiy[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries play an important role in determining the physical properties of materials. With respect to diffusion, extended strain fields localized at GBs can modify atomic transport along GBs. In order to understand the effect of strain on GB diffusion in more detail, the evolution of strain along GBs under mechanical treatment is investigated. For this purpose, a Cu bi-crystal containing a sigma 5(310) GB was fabricated by a modified Bridgman technique, followed by annealing at 800 °C. The surface was mirror-liked polished subsequently followed by FIB lamella target preparation of the GB in cross-sectional view. The elastic strain along and around the GB was measured on a nanometer scale, using nano-beam diffraction patterns (NBDPs) acquired using a 1 nm STEM probe with grains oriented in zone axis conditions. A custom written code was employed to extract the strain maps. On the atomic scale, the strain was characterized using geometrical phase analysis applied to high resolution STEM images confirming the results obtained by NBDP. The analysis was finally extended to deformed samples.

MM 42.4 Wed 16:30 C 130

Unfolding structural features of NaNbO3 using atomic resolution 4D-STEM — •Hui Ding[1], Yu Huang[2], Mao-Hua Zhang[3], Jing-Feng Li[2], and Christian H. Liebscher[1] — [1]Structure and Nano- / Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]School of Materials Science and Engineering, Tsinghua University, Beijing, China — [3]Department of Materials Science and Engineering, Penn State University, University Park, USA

As one of the most promising lead-free antiferroelectrics, $NaNbO_3$ suffers from irreversibility of the phase transition, limiting further application in electronic devices. Understanding the structural complexity and establishing a well-defined structure-property relationship of $NaNbO_3$ is of great importance for targeted tailoring of its functionality.

Here, we employ atomic resolution HAADF-STEM and 4D-STEM to probe the local atomic structure of $NaNbO_3$ thin films resolving the Nb, Na and O sublattices simultaneously. Reconstructed differential phase contrast STEM images indicate either the coexistence of P4bm (tetragonal) and $P2_1$ma (orthorombic) phases, instead of the intrinsic Pbcm phase, or the formation of a new hybrid phase. In particular, the O columns form a zig-zag pattern along the Nb columns in the (001) plane due to O octahedral tilting, which is the characteristic of the $P2_1$ma phase. However, an alternating contrast of the Na columns, characteristic for the P4bm phase, is observed and confirmed by 4D-STEM image simulations.

MM 42.5 Wed 16:45 C 130

Machine learning-enabled tomographic imaging of chemical short-range order in Fe-based alloys — •Yue Li and Baptiste Gault — Max-Planck Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Chemical short-range order (CSRO), describing preferential local ordering of elements within the disordered matrix, can change the mechanical and functional properties of materials. CSRO is typically characterized indirectly, using volume-averaged (e.g. X-ray/neutron scattering) or through projection microscopy techniques that fail to capture the complex, three-dimensional atomistic architectures. Quantitative assessment of CSRO and concrete structure-property relationships have remained so far unachievable. Here, we present a machine-learning enhanced approach to break the inherent resolution limits of atom probe tomography to reveal three-dimensional analytical imaging of the size and morphology of multiple CSRO. We showcase our approach by addressing a long-standing question encountered in a body-centred-cubic Fe-18Al and Fe-19Ga (at.%) alloy that sees anomalous property changes upon heat treatment, supported by electron diffraction and synchrotron X-ray scattering techniques. The proposed strategy can be generally employed to investigate short/medium/long-range ordering phenomena in a vast array of materials and help design future high-performance materials.

MM 42.6 Wed 17:00 C 130

TESCAN 4D-STEM for Multimodal Characterization of Challenging and Interesting Specimens — Lars-Oliver Kautschor[1] and •Robert Stroud[2] — [1]TESCAN GmbH. Zum Lonnenhohl 46, Dortmund — [2]TESCAN USA, 765 Commonwealth Dr #101, Warrendale, PA 15086, USA

The all-new TESCAN TEM solution: TESCAN TENSOR - the world*s first Integrated, Precession-assisted, Analytical 4D-STEM will be presented. Designed from the ground up TESCAN TENSOR*s quality throughput, and robustness of 4D-STEM acquisition, analysis, and processing has been optimized with state-of-the-art technologies, such as Precession Electron Diffraction (PED), 4D-STEM computing and visualization, electrostatic beam blanking, and ultra-high vacuum at the specimen area. Additionally, TESCAN TENSOR features real-time, automated data analysis and processing, which empowers an unprecedented level of system accessibility, utilization, and productivity. The methodology behind this advanced (electron diffraction) microscope will be explained as the solution of choice for a range of nanoscale applications.

MM 42.7 Wed 17:15 C 130

Micro-CT goes multimodal - 3D elemental analysis with new the SPECTRAL CT, — •Lars-Oliver Kautschor — TESCAN GmbH. Zum Lonnenhohl 46, Dortmund

X-ray micro-computed tomography (micro-CT) has opened new avenues of research and understanding. It is now recognized as an essential technique for non-destructive 3D imaging. Extending the technique to the temporal regime, through time-resolved 3D imaging (or 4D imaging), provides a new route to better and more complete understanding of materials evolution, facilitating in situ investigations ranging from mechanical deformation to fluid flow in porous materials. With the new SPECTRAL CT, TESCAN offers the possibility to perform elemental analysis inside your sample none-destructively. In this talk we explore the general technique of micro-CT as well as the advantages of the new SPECTRAL.

Topical Talk MM 42.8 Wed 17:30 C 130

Unsupervised Machine Learning Analysis for Electron Microscopy Datasets — •Mary Scott — Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, CA 94720, USA — National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA 94720, USA

Electron microscopy is the characterization method of choice to observe local atomic-scale and microstructural features within materials that play a critical role in material performance. Recently developed high frame rate electron detectors acquire diffraction patterns from nanoscale regions at frame rates of 100 kHz, an approach that enables multimodal analysis from the same dataset to create maps of crystal orientation, strain, and more. This method, termed 4D-STEM, creates datasets can contain tens of thousands of diffraction patterns from heterogeneous structural regions. The large datasets cannot be analyzed manually, and lack of prior knowledge of the crystal structure of diverse samples limits the application of supervised automated approaches, motivating the development of unsupervised analysis. Here I will overview implementation of an automated, unsupervised clustering pipeline for 4D-STEM data, emphasizing the importance of input data representation. Futhermore, I will describe an ensemble approach to generate more stable clustering results. This type of unsupervised data analysis pipeline is an important step towards incorporating rapid 4D-STEM analysis into material discovery and design efforts, particularly when evaluating defect-rich and disordered materials.

MM 43: Data Driven Material Science: Big Data and Workflows V

Time: Wednesday 15:45–18:00 Location: C 243

MM 43.1 Wed 15:45 C 243

The MALA Package - Transferable and Scalable Electronic Structure Simulations Powered by Machine Learning — •Lenz Fiedler and Attila Cangi — Helmholtz-Zentrum Dresden-Rossendorf / CASUS

Interactions between electrons and nuclei determine all materials properties, and modeling these interactions is of paramount importance to pressing scientific questions. However, even with the most advanced electronic structure tools, such as density functional theory (DFT), electronic structure simulations are usually restricted to a few thousand atoms.

Machine-learning DFT (ML-DFT) tackles this challenge by providing rapid access to observables of interest. Most current ML-DFT methodologies focus on the mapping between ionic configurations and scalar observables, rather than a full prediction of electronic structure. The Materials Learning Algorithms (MALA) python package addresses this gap, by providing a user-friendly framework to construct ML-DFT models that give access to a range of electronic structure observables, such as the electronic density, DOS and total free energy. The usefulness of these models across phase boundaries [1], multiple length scales [2] and temperature ranges [3] has been amply demonstrated. In this talk, a general introduction to the framework along with its computational properties and capabilities is given.

[1] J. A. Ellis *et. al*, Phys. Rev. B, 2021, **104**, 035120 ** [2] L. Fiedler *et. al*, npj Comput. Mater., 2022, **9**, 115

[3] L. Fiedler *et. al*, Phys. Rev. B, 2023, **108**, 125146

MM 43.2 Wed 16:00 C 243

A robust, simple and efficient algorithm to converge GW calculations — •Max Grossmann, Malte Grunert, and Erich Runge — Theoretische Physik I, TU Ilmenau, Germany

In the era of high-throughput computation for materials science and machine learning, the demand for heuristics and efficient convergence schemes in ab initio calculations has become essential to speed up computational workflows. A prime example of computationally demanding ab initio material-science calculations is the GW method, which is crucial for accurate band gap predictions and the subsequent computation of dielectric functions using TDDFT/BSE. The main hurdle within GW calculations lies in the convergence of two interdependent parameters in the dynamic screening W which must be optimized simultaneously. To overcome this obstacle we introduce a straightforward, "cheap first, expensive later" coordinate-search algorithm, which is tested against a commonly used state-of-the-art method on a diverse dataset of 50 semiconducting and insulating solids. Additionally, the practical independence between the **k**-point grid and parameters in W is checked using both algorithms on five different **k**-meshes of increasing density for all investigated materials, starting at $\mathbf{\Gamma}$-only calculations. The results show how to converge GW calculation in a robust, simple and efficient way.

MM 43.3 Wed 16:15 C 243

FAIR Data Management for Computational Materials Science using NOMAD — •Luca M. Ghiringhelli[1], Joseph F. Rudzinski[2], José M. Pizarro[2], Nathan Daelman[2], and Silvana Botti[3] — [1]Department of Materials Science and Engineering, Friedrich-Alexander-Universität, Erlangen-Nürnberg — [2]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin, Berlin — [3]RC-FEMS and Faculty of Physics, Ruhr University Bochum, Bochum

NOMAD [nomad-lab.eu][1, 2] is an open-source data infrastructure for materials science data. Originally built as a repository for DFT calculations, NOMAD has been extensively developed over the past 2 years to support a wide range of both computational and experimental data. Additionally, NOMAD now includes a general workflow support that not only streamlines data provenance and analysis but also facilitates the curation of AI-ready datasets. This talk will demonstrate how these features, along with NOMAD's adherence to the FAIR principles (Findability, Accessibility, Interoperability, Reusability), provide a powerful framework for enhancing data utility and discovery. I will highlight how this FAIR-compliant perspective distinguishes NOMAD from other Big-Data infrastructures, e.g., allowing users to specify their data quality needs. Finally, I will provide an outlook of NOMAD's potential for creating a cohesive, interconnected, and economical scientific data landscape.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).

[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 43.4 Wed 16:30 C 243

A many-body framework for long-range interactions in atomistic machine learning — •Kevin Kazuki Huguenin-Dumittan, Philip Robin Loche, and Michele Ceriotti — EPFL, Lausanne, Switzerland

Many properties of matter, from chemical bonds to the band structure in solids, arise from the quantum nature of electrons. Accurate atomistic modeling of such systems thus requires the use of quantum approaches, which can computationally become prohibitively expensive compared to their classical counterparts. Machine learning based approaches have seen a surge in interest over the past decade to bridge the gap between the two worlds by providing near-quantum accuracy at a cost scaling similarly to classical methods. One systematic source of error in most such models is the assumption of locality, which neglects important long-range interactions ranging from electrostatics to more complex effective interactions between macromolecules. In this talk, we present a long-range framework that is a significant improvement over the previously introduced LODE descriptors, which (1) scales effectively linearly with system size, (2) captures a broad family of long-range interactions beyond the Coulomb potential, (3) can systematically generate many-body features beyond just pair potentials and (4) smoothly and fully integrates with preexisting machine learning frameworks with little extra effort including the computation of gradients or equivariant models for tensorial properties.

MM 43.5 Wed 16:45 C 243

Automated prediction of Fermi surfaces from first principles — •Nataliya Paulish[1], Junfeng Qiao[2], and Giovanni Pizzi[1,2] — [1]Paul Scherrer Institut (PSI), Villigen, Switzerland — [2]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Knowing the shape of the Fermi surface (FS) and the energy dispersion in its vicinity is crucial to understand the electronic properties of materials and identify materials relevant for applications. Experimental methods to measure FSs are very expensive and time-consuming, and accurate theoretical predictions would help to get deeper insights from the experimental data. Direct first-principles calculations of the FS, requiring very dense sampling in reciprocal space, are thus limited by the computational cost. To accelerate the calculations, we use interpolation with Maximally Localized Wannier Functions (MLWFs), powered by our new method that allows fully automated calculation of MLWFs [1]. We first validate the numerical approach by comparing our simulation results with literature data for de Haas-van Alphen (dHvA) oscillation frequencies and investigate the main sources of numerical errors. We then use our high-throughput setup, with our code implemented as an AiiDA [2] workflow, to create a large database of Fermi surfaces and dHvA oscillation frequencies of 3D inorganic metals, starting from high-symmetry systems.

[1] J. Qiao *et al.*, npj Comput. Mater. 9, 208 (2023)

[2] S. P. Huber *et al.*, Scientific Data, 7, 300 (2020)

15 min. break

MM 43.6 Wed 17:15 C 243

Accurate and Efficient Protocols for High-Throughput Computational Materials Science — •Gabriel M. Nascimento[1], Flaviano José dos Santos[2], Marnik Bercx[2], Davide Grassano[1], Giovanni Pizzi[2], and Gabriel de Miranda Nascimento[1,2] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Laboratory for Materials Simulations (LMS), Paul Scherrer Insititute, Villigen, Switzerland

Advances in simulation methods and workflow engines, and an ever-increasing computational power have enabled the paradigm change in computational materials science of high-throughput (HT) discovery. A significant challenge in these efforts is to automate the choice of parameters in simulation codes, where a consistent balance of accuracy and computational cost is required. We propose a rigorous methodology to assess the quality and sensitivity of self-consistent density-functional theory (DFT) calculations with respect to smearing and Brillouin zone sampling of 2D and 3D crystalline compounds. Our results enable the construction of unified protocols for the choice of parameters that guarantee k-point sampling convergence and control of entropic systematic errors for calculations within most classes of materials, while minimizing the required overall wall time. These protocols are integrated into automated workflows for DFT calculations using QUANTUM ESPRESSO, accessible through the open-source AiiDA framework. This work streamlines access to state-of-the-art computational frameworks, fostering HT research and supporting the development of computational materials databases.

MM 43.7 Wed 17:30 C 243

Defect Phase Diagrams for Grain Boundaries in Mg: Automized workflows for chemical trends — •PRINCE MATHEWS[1], REBECCA JANISCH[2], JÖRG NEUGEBAUER[1], and TILMANN HICKEL[1,3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]ICAMS, Ruhr Universität Bochum, Germany — [3]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

The design of lattice defects is a crucial component for processing tailored materials as they control the mechanical properties and corrosion behavior. In order to achieve this, the framework of defect phase diagrams is a powerful and knowledge-based design strategy, which can be used to manipulate defect phases using defect-property relationships. Defect phase diagrams use the chemical potential as the key variable as it has the same value at the defect as well as in the adjacent bulk. With pyiron, an integrated development environment for computational materials science, an automatic workflow has been developed for calculating defect phase diagrams for binary systems using ab-initio simulations. The workflow is used for the example of Ga and Ca segregation to Σ7 [0001] 21.78° (sym. plane 12-30) Mg grain boundaries. Chemical trends for the relative stability of different atomic configurations at the grain boundaries are derived. Connecting the workflow with experimental datasets, a good agreement has been confirmed. The advantages of automized workflows for the defect phase diagrams is then demonstrated for the extension of the considerations to finite temperatures and free energies calculated within the quasi-harmonic approximation.

MM 43.8 Wed 17:45 C 243

High-level hybrid workflow-based approach for characterizing magnetocaloric materials: concurrent computational and experimental validation — •SIMON BEKEMEIER[1], ALISA CHIRKOVA[1], and CHRISTIAN SCHRÖDER[1,2] — [1]Hochschule Bielefeld - University of Applied Sciences and Arts — [2]Faculty of Physics, Bielefeld University

Processing of expanding experimental and computational datasets often requires multiple tools applied in a sequence before the main result is retrieved. Data treatment, its transfer between different tools and sharing are key points in nowadays materials development and digitalization processes. A study of magnetocaloric materials produces a moderate size dataset, from which certain values need to be calculated (ΔS, magnetic entropy change). Obtaining it from first principles requires several computational steps, with the output of the previous step transferred to the next one. In this work, a workflow for the ΔS-calculation from both experimental and theoretical data is developed. The computational tools are accessed through the pyiron©IDE that includes atomistic simulations using density functional theory as well as newly implemented CINOLA spin-dynamics and magnetic transition evaluation from thermodynamics. As a proof of concept, we show results for Ni and Gd exhibiting a second-order magnetic phase transition and for representative model materials with a first-order phase transition. Our approach has an advantage of the acceleration and automatization of the data transformation and treatment within a single study; furthermore, it offers experimentalists a convenient option to perform powerful simulations on their own.

MM 44: Developement of Calculation Methods II

Time: Wednesday 15:45–18:00 Location: C 264

MM 44.1 Wed 15:45 C 264

FAIR Data Quality Metrics in NOMAD — •NATHAN DAELMAN[1], JOSEPH F. RUDZINSKI[1], JOSÉ M. PIZARRO[1], LUCA M. GHIRINGHELLI[2], and SILVANA BOTTI[3] — [1]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin, Berlin — [2]Department of Materials Science and Engineering, Friedrich-Alexander-Universität, Erlangen-Nürnberg — [3]RC-FEMS and Faculty of Physics, Ruhr University Bochum, Bochum

The FAIR principles (Findable, Accessible, Interoperable, Reusable) serve as a reference for assessing the quality of data storage and publication [1]. NOMAD [nomad-lab.eu][2, 3] is an open-source data infrastructure for materials science data that is built upon these principles.

In this presentation, I will demonstrate the interplay between high-quality data and knowledge using the functionalities provided by NOMAD and with DFT as an example case. In particular, I will showcase the dynamic and flexible metadata framework, designed for a clearer, more customizable navigation of the zoo of density functionals. I will then show how precision and accuracy metrics are represented within this framework, and how they can be linked to benchmark datasets. Finally, I will present a brief outlook on the future of NOMAD as a platform that fosters an interconnected research community and engaged scientific discourse.

[1] Wilkinson, M. D. *et al.*, Sci. Data **3**, 160018 (2016).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).
[3] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).

MM 44.2 Wed 16:00 C 264

Machine-learning interatomic potentials with beyond-DFT accuracy: application to covalent-organic frameworks — •YUJI IKEDA, AXEL FORSLUND, and BLAZEJ GRABOWSKI — University of Stuttgart, Stuttgart, Germany

Covalent-organic frameworks (COFs) are nanoporous crystalline materials formed by strong covalent bonds of organic secondary building units composed mostly of light elements like C, N, O, H, etc. Most COFs are quasi-two-dimensional materials with layers interacting with van der Waals (vdW) forces. It is fascinating to investigate COFs using machine-learning interatomic potentials (MLIPs) because of their capability to access, e.g., long time- and length-scales in molecular-dynamics (MD) simulations. To simulate vdW materials, MLIPs should be trained by data including the vdW interaction. Such data are typically prepared with vdW-DFT functionals. These vdW-DFT functionals are however essentially semi-empirical in the sense that their parameters are fitted to show agreement with experiments, and hence they imply concerns about transferability. Our solution is to consider training data obtained from post-Hartree-Fock (HF) methods such as the coupled-cluster (CC) methods, which are non-empirical and have beyond-DFT accuracy. Using MLIPs trained on the beyond-DFT data, we demonstrate the calculation of structural properties of COFs.

MM 44.3 Wed 16:15 C 264

Kinetic Modeling of Stripes, Surfaces, and Solids Using the kmos3 Framework — •MARTIN DEIMEL[1], ADITYA SAVARA[2], KARSTEN REUTER[1], and SEBASTIAN MATERA[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Oak Ridge National Laboratory, Tennessee, United States

Kinetic Monte Carlo (KMC) simulations have attracted growing attention over the years for the modeling of diverse surface or bulk processes, e.g., crystal growth, catalytic reactions, or diffusion in solids. We introduce the open-source Python package kmos3 for lattice KMC, the third revision of the original kmos package.[1] Being based on the rejection-free variable step size algorithm, kmos3 acts as a flexible code generator framework, creating model-specific efficient Fortran code which is subsequently compiled to a Python callable library. Using different prototypical models, we demonstrate the usage of kmos3. The different available backends, which target different classes of models, will be analyzed in terms of their performance with respect to model complexity and system size. Finally, we will discuss how to speed up KMC simulations of problems with time-scale separation using the implemented acceleration algorithm.[2]

[1] M. Hoffmann, S. Matera, and K. Reuter, Comput. Phys. Commun. **185**, 2138 (2014).
[2] M. Andersen, C. Plaisance, and K. Reuter, J. Chem. Phys. **147**, 152705 (2017).

MM 44.4 Wed 16:30 C 264

Extracting Gibbs free energies from local composition fluctuations in atom probe data — Jianshu Zheng[1], Rüya Duran[1], Marvin Poul[2], Guido Schmitz[1], and •Sebastian Eich[1] — [1]Institute for Materials Science, University of Stuttgart, Germany — [2]Department of Computational Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

While thermodynamic fluctuation theory has been applied to liquids for decades to obtain Gibbs free energies from local composition fluctuations, the present work extends this theory to solids by considering an additional elastic work term. This theory is firstly verified via atomistic embedded-atom simulations in an exemplary Cu–Ni system using Monte Carlo techniques. Composition fluctuations, which are evaluated for various-sized subvolumes, reveal a systematic dependence on the size of the evaluation volume, but extrapolation to an infinitely large subvolume leads to perfect agreement with the prediction by the extended theory. Thus, recovering Gibbs free energies becomes indeed possible also in solids. In a second step, this method is now applied to experimental atom probe tomography (APT) data with high chemical and spatial resolution, enabling the analysis of local composition fluctuations. From these data, the Gibbs free energy is recovered and remarkable agreement is found between our approach and the latest CALPHAD representation of the miscibility gap. This methodology is therefore believed to efficiently improve the accuracy of thermodynamic information (e.g. miscibility gap, mixing/demixing tendencies, critical solution temperature) from direct APT measurements.

MM 44.5 Wed 16:45 C 264

Improving the Diversity of Transition State Searches with On-the-fly Learned Biasing Potentials — •Nils Gönnheimer[1,2], King Chun Lai[1], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Institut der MPG Berlin — [2]Universität Bayreuth

Constructing reaction networks of reaction pathways is fundamental for long-timescale simulations and the theoretical analysis of complex chemical processes. A common approach involves using minimum mode following (MMF) methods to identify these reaction pathways, and especially transition states (TSs), on potential energy surfaces (PESs). However, MMF methods may miss essential reaction pathways due to their tendency of converging towards a limited set of transition states, even when simulations are repeated with different starting conditions. Herein, we address this limitation by introducing a biasing potential which modifies the PES based on on-the-fly gathered information. The bias drives the TS search algorithm away from known TSs and therefore increases the diversity of the outcome. We demonstrate the impact of the on-the-fly generated bias on the MMF method by showing the change of basins of attraction for first-order saddle points within a benchmark 2D PES. Furthermore, we will illustrate the effect of the bias on the diversity of identified TSs during a restricted number of TS searches for the self-diffusion of a heptamer on a Pt(111) surface.

15 min. break

MM 44.6 Wed 17:15 C 264

Kernel Charge Equilibration: Machine Learned Interatomic Potentials With Full Long-Range Electrostatics — •Martin Vondrak[1], Johannes T. Margraf[1,2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Machine learning (ML) interatomic potentials 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 system's structure and its physical properties. To this end, state-of-the-art models typically represent chemical structures in terms of local atomic environments. This inevitably leads to the neglect of long-range interactions (most prominently electrostatics) and non-local phenomena (e.g. charge transfer), resulting in significant errors in the description of polar molecules and materials (particularly in non-isotropic environments). To overcome these issues, we recently proposed an ML framework for predicting charge distributions in molecules termed Kernel Charge Equilibration (kQEq) [1]. Here, atomic charges are derived from a physical model using environment-dependent atomic electronegativities. In this contribution, strategies for creating kQEq interatomic potentials are discussed, including the combination of short-ranged Gaussian Approximation Potentials with kQEq.

[1] M. Vondrak, K. Reuter, and J.T. Margraf, J. Chem. Phys. **159**, 054109 (2023).

MM 44.7 Wed 17:30 C 264

Sampling-free computation of finite temperature material properties in isochoric and isobaric ensembles using the mean-field anharmonic bond model — •Raynol Dsouza[1], Marvin Poul[1], Liam Huber[2], Thomas D. Swinburne[3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, 40327, Germany — [2]Grey Haven Solutions, Victoria, BC, Canada — [3]Aix-Marseille Universite, CNRS, CINaM UMR 7325, Campus de Luminy, Marseille 13288, France

The recently introduced mean-field anharmonic bond model has shown remarkable accuracy in predicting finite temperature free energies for certain potential models of fcc crystals without thermodynamic sampling. In this work, we extend the model to treat modern machine learning potentials in both isochoric and isobaric ensembles. Testing against molecular dynamics simulations of Al and Cu, we find meV/atom accuracy in free energies up to the melting temperature under typical operating pressures, with similar accuracy for the thermal expansion. Our sampling-free estimation is universally superior to the quasi-harmonic approximation for a computational cost that is nearly two orders of magnitude lower and many orders of magnitude more efficient than thermodynamic integration. We discuss applications of the method in modern computational materials science workflows.

MM 44.8 Wed 17:45 C 264

Exploring Alternative Dispersion Corrections for the BEEF-vdW Functional — •Elisabeth Keller[1], Johannes T. Margraf[1], Volker Blum[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Department of Mechanical Engineering and Materials Science, Duke University, Durham, United States

The BEEF-vdW exchange-correlation functional was developed as a general purpose functional for chemistry and condensed matter physics. As such, BEEF-vdW gives a balanced description for molecular and solid-state systems, making it particularly well-suited to investigate surface science and catalytic processes. However, the use of a nonlocal vdW functional to describe dispersion interactions makes BEEF-vdW computationally expensive and difficult to incorporate in many electronic structure codes. In this work, we therefore explore the use of different alternative dispersion corrections to emulate the general applicability of BEEF-vdW in the FHI-aims code. We discuss the impact that the choice of dispersion correction (TS-vdW, MBD, MBD-NL, XDM) has on the accuracy and computational demand of BEEF-vdW for molecular, surface and solid-state systems.

MM 45: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials IV

Time: Wednesday 15:45–17:00 Location: C 230

MM 45.1 Wed 15:45 C 230

Ab initio insights into compositional dependence of TWIP and TRIP barriers of Ti-alloys — •David Holec[1], Johann Grillitsch[1], José Neves[2], and Thomas Klein[2] — [1]Department of Materials Science, Montanuniversität Leoben, 8700 Leoben, Austria — [2]LKR Light Metals Technologies, AIT Austrian Institute of Technology, 5282 Ranshofen, Austria

Advanced manufacturing, such as additive manufacturing, is a promising concept for a more material-efficient production route of components with complex shapes. However, this new technology also brings new challenges such as different microstructures and compositions. In this contribution, we will present a fundamental study on the impact of alloying species on transformation barriers in Ti-alloys. We employ ab initio methods to calculate the potential energy surface (PES) for a bcc-to-hcp transformation as a model for transformation-induced plasticity (TRIP), as well as stacking fault energies together with their barriers for different twinning mechanisms as a measure of the twinning-induced plasticity (TWIP). We present strategies for evaluating the alloying impact on those measures using a thermodynamics-based statistical averaging of various local configurations.

MM 45.2 Wed 16:00 C 230

Dislocation-mediated non-basal plasticity in topologically close-packed phases — •Zhuocheng Xie[1], Martina Freund[1], Wei Luo[1], Christina Gasper[1], Pei-Ling Sun[1], Siyuan Zhang[2], and Sandra Korte-Kerzel[1] — [1]Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, Kopernikusstraße 14, 52074 Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany

Topologically close-packed (TCP) phases exhibit great promise as high-temperature structural materials, however, their notorious brittleness at room temperature limits their applications. The dislocation motion mechanisms in these complex alloys, especially on non-basal/{111} planes, remain poorly understood. We perform atomistic simulations to elucidate the deformation mechanisms of TCP phases and complement with experimental observations from nanomechanical testing at room temperature. Dislocation glide and cross-slip mechanisms among newly identified {11n} slip planes in cubic Laves phases and associated minimum energy paths are determined. Additionally, we unveil a new non-basal slip mechanism, namely the formation of (1-105) stacking fault by partial dislocation glide with a Burgers vector of 0.07[-5502], in μ-phases. This comprehensive exploration of dislocation dynamics not only contributes to a fundamental understanding of TCP phases but also paves the way for tailored design strategies to enhance their mechanical properties at room temperature.

MM 45.3 Wed 16:15 C 230

Anomalous brittleness of iridium: Atomistic insights from DFT and ACE simulations — •Minaam Qamar, Matous Mrovec, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr University Bochum, Germany

The anomalous brittle nature of face-centered cubic (fcc) metal iridium has puzzled researchers for decades. We investigated fracture mechanisms in Ir using atomistic simulations based on density functional theory (DFT) and the atomic cluster expansion (ACE). ACE is a data-driven interatomic potential with a formally complete basis that can reach quantum accuracy while remaining highly computationally efficient. Both transgranular cleavage in perfect bulk and intergranular fracture along grain boundaries were examined. Detailed computational tensile tests for several grain boundaries were performed in parallel for Ir and Cu, which can be considered a prototypical ductile fcc metal. Subsequently, ACE parametrizations for both metals were employed in large-scale atomistic simulations of various fracture scenarios at finite temperatures and different loading conditions. We will present results of the simulations and discuss new insights into the intrinsic fracture behavior of Ir.

MM 45.4 Wed 16:30 C 230

Parameterising dislocation dynamics in Ni-based superalloys from atomistic simulations — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry CV4 7AL, UK

Ni-based superalloys are important materials for high temperature applications. Nanoscale precipitates in their microstructure hinder dislocation motion, which results in an extraordinary strengthening effect at elevated temperatures. In the present work, we parameterise the motion of edge dislocations in pure face-centred cubic (FCC) Ni, which we use to represent an idealized γ phase in Ni-based superalloys. Molecular dynamics (MD) simulations with classical effective potentials were used to obtain edge dislocation trajectories, and the parameters of equations of motion were then fitted using Differential Evolution Monte Carlo (DE-MC) within a Bayesian framework. The reduced model accounts for dislocation-dislocation and dislocation-precipitate interactions, and the fitting procedure yields physically meaningful parameters. Using DE-MC sampling makes it possible to obtain parameter distributions and propagate uncertainties through the model, quantifying the uncertainty in its predictions: the dislocation positions and velocities. This work serves as a first step towards building a more comprehensive surrogate model that can describe the deformation behaviour of Ni-based superalloys, where the parameterisation approach employed here can offer a quantitative measure of the effect of precipitates on dislocation dynamics in these materials.

MM 45.5 Wed 16:45 C 230

Dislocation Crack 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 single crystalline Tungsten at low temperature is critically influenced by its microstructure. Understanding the underlying crack-microstructure interactions is therefore necessary to model and predict materials failure. In order to gain insight into the interactions of dislocations with crack tips, large-scale atomistic simulations are carried out. Screw dislocations are placed in the vicinity of a strain-controlled crack. In various crack systems screw dislocations that are attracted towards the crack tip have a strong tendency to cross-slip at the crack tip and glide along the crack front. Driving forces for this phenomenon as well as implications for fracture behaviour shall be discussed in this contribution.

MM 46: Structurally and Chemically Complex Alloys (joint session MM/KFM)

Time: Wednesday 17:15–18:00 Location: C 230

MM 46.1 Wed 17:15 C 230

Synthesis and atomic transport properties in pseudo-binary ordered B2 aluminides — •Mohan Muralikrishna Garlapati[1], Christian H. Liebscher[2], Murty B.S.[3], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Muenster, 48149-Muenster, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, 600036-Chennai, India.

The present study highlights a novel alloy design of HEAs to fabricate fully ordered pseudo-binary multicomponent and ordered aluminides and is focused on the underlying diffusion behaviour. Microstructure and sublattice ordering in the multicomponent alloys starting from binary to hexanary B2 aluminides are studied. A radiotracer technique using the 57Co, 59Fe, 54Mn, 63Ni and 65Zn radioisotopes is employed to measure the diffusion rates of individual elements. Diffusion in the multicomponent (n>4) B2 ordered alloys is found to be enhanced in comparison to stoichiometric binary AlNi. However, the addition of Co or Fe to AlNi slows down (Co) or enhances (Fe) the diffusion rates. The measured diffusivities are compared to the literature data and the effect of chemical complexity and the B2 ordering on diffusion are discussed.

MM 46.2 Wed 17:30 C 230

Short range order in compositionally complex NiCoMnTi alloys — David Koch[1], Benedikt Beckmann[1], Oleh Ivasko[2], Martin von Zimmermann[2], Oliver Gutfleisch[1], and •Wolfgang Donner[1] — [1]Institute of Materials Science, Technical University of Darmstadt , 64287 Darmstadt, Germany — [2]Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

Analyzing the chemical order in compositionally complex alloys can be challenging and may become complicated by low elemental contrast. One such compositionally complex material is the all-d-Heusler alloy NiCoMnTi. These alloys exhibit a tunable magneto-structural phase transition, where the high-temperature phase has a long-range B2 structure that can be adjusted through proper thermal treatment. The typical long-range $L2_1$ structure found in classical p-metal Heusler alloys cannot be stabilized. In this report, we present data on short-range order in this system, which can be probed through diffuse X-ray scattering. To achieve this, we grew single crystals via abnormal grain growth and conducted synchrotron high-energy X-ray diffraction experiments to obtain high-quality diffuse scattering data. This data was then reconstructed into reciprocal space maps for interpretation.

MM 46.3 Wed 17:45 C 230

Mechanical Alloying of High-Entropy Alloys: Insights from Molecular Dynamics Simulations — •Marie Charrier, Yulia Klunnikova, and Karsten Albe — Technical University of Darmstadt, Materials Modelling Division, Otto-Berndt Straße 3, 64206 Darmstadt, Germany

Mechanical alloying is a promising technique for producing high-entropy alloys. In this work, we explore intermixing processes and the formation of the solid solution starting from principal elements Co, Fe, Ni, Cr and Al in their respective lattice structures.

Severe plastic deformation is mimicked in Molecular Dynamics simulations by cyclic compressive loading of nanocrystalline samples inducing a quasi-hydrostatic stress state. The influence of grain orientation, grain size and temperature on structural evolution and chemical mixing is investigated. The structural and chemical complexity is increased by varying interfaces (from planar, bicrystalline to multiple, randomly oriented grains) and the number of components, respectively.

Independent of the starting configuration, we observe grain refinement and an HCP/BCC-FCC phase transformation within a few cycles, while chemical homogeneity is reached only at higher strains. These processes strongly depend on temperature and grain size, while the grain orientation plays a minor role. The final structures exhibit a large number of defects, in agreement with experimental observations. In general, the results provide atomic level insights into the mechanisms of mechanical alloying.

MM 47: Poster DS (joint session DS/MM/O)

Time: Wednesday 17:00–19:00 Location: Poster B

MM 47.1 Wed 17:00 Poster B

Tailoring Ti3C2 MXenes towards the Oxygen Evolution Reaction — •Aline Alencar Emerenciano and Michelle Browne — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Ti3C2 MXenes are promising materials for water splitting due to their high conductivity, hydrophilicity, and good mechanical properties when compared to other 2D-nanomaterials [1]. The possibility of tailoring MXenes in terms of functional groups, flake size/shape, presence of defects, and surface area makes them excellent candidates to be hybridized with transition metal oxides. MXenes/TMO catalysts can provide synergetic properties such as high conductivity in combination with active sites for Oxygen Evolution Reaction (OER). To reduce the mass loading by increasing the intrinsic activity and stability of MXenes, the surface functionalization and surface area must be controlled. In this work, in situ generated HF was utilized to remove Al-elements for the production of Ti3C2. Synthesis protocols utilizing different concentrations of HCl were investigated to evaluate the flake quality in terms of functional groups distribution, flake size towards the existence of multilayered and delaminated nanoflakes, as well as the concentration of pin-roles on their surface. Overall, this work provides a better understanding in how HCl concentration can influence the MXenes contribution in hybrid electrocatalysts considering functional groups distribution and presence of defects.

1.Zhang, C. J. et al. Adv. Mater. 29, 1-9 (2017).

MM 47.2 Wed 17:00 Poster B

Chemical functionalisation of CuCo(2)-LDH on V(2)CT(x) for the oxygen evolution reaction — •Bastian Schmiedecke and Michelle Browne — Helmholtz-Zentrum Berlin, Berlin, Germany

MXenes, known for their exceptional surface area and high conductivity, serve as excellent catalyst supports, enhancing electrocatalytic performance in the oxygen evolution reaction (OER). Layered double hydroxide (LDH) materials, though promising for the OER, lack conductivity to ensure easy charge transfer during electrochemical processes. While, research on LDH materials has developed rapidly, there remains a high demand for refining the strategic combination of LDH with two dimensional (2D) materials, such as MXenes, which can significantly improve the water oxidation performance of LDH materials by inducing high conductivity, hydrophilicity and surface area.

This study introduces a hybrid catalyst, CuCo2-LDH grown on delaminated vanadium carbide (V(2)CT(x)) nanosheets to enhance the OER performance. The synthesized CuCo(2)-LDH@V(2)CT(x) electrocatalyst exhibited excellent activity with an overpotential of 289 mV at a catalytic current density of 10 mA cm-2 with a Tafel slope value of 74 mV dec-1. Furthermore, slight performance improvements were observed after 12 h of continuous operation. We propose that the enhanced performance is attributed to the conductivity of V(2)CT(x) and its synergistic interaction with CuCo(2)-LDH, effectively minimizing aggregation, exposing more active sites. This work demonstrates the significant potential of combining LDH-based nanomaterials with V(2)CT(x) MXene for energy conversion applications.

MM 47.3 Wed 17:00 Poster B

Analysis of polarization dependent IR spectra of thin films — •Karsten Hinrichs[1], Andreas Furchner[2], Fatima Akhtar[2], Norbert H. Nickel[2], and Jörg Rappich[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Application Laboratories Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH 14109 Berlin, Germany

The interpretation of bands in polarization dependent infrared (IR) spectra of thin films is addressed. Several examples such as an isotropic polymer film and functionalized silicon surfaces will be discussed as case studies. It will be shown that the observed vibrational band properties depend on the measurement geometry, the film thickness, the materials dielectric functions, as well as the direction of the probing electromagnetic fields. Comparative Density Functional Perturbation Theory (DPFT) - calculations are used for analysis. The financial support by the Europäischer Fonds für regionale Entwicklung by EFRE 1.8/13 and ProFIT 10185407 as well as the Federal Ministry of Education and Research and the project CatLab (03EW0015A/B) is acknowledged.

MM 47.4 Wed 17:00 Poster B

Focused-Ion-Beam induced Defect Emission in Hexagonal Boron Nitride

— •Felix Schaumburg, Dominik Kaczmarek, David Plitt, Martin Geller, Günther Prinz, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Defects in the wide bandgap material hexagonal boron nitride (hBN) exhibit single-photon emission at room temperature (RT) [1]. We used the gallium ion beam of a focused ion beam (FIB) to generate ensembles of defects that we associated with boron vacancies having a photoluminescence emission exceeding 800 nm [2]. After irradiation isolated point defects can also be found next to the irradiated areas. We show that our created defects exhibit a bright RT emission, an almost sublinear power dependence commonly associated with a two-level system and an increasing signal, a decreasing full with at half maximum (FWHM), and a minimal shift to lower wavelengths at lower temperatures. Our results show, that we can generate bright emitters in hBN by Ga-ion treatment that are in a wavelength range of up to 800 nm. Our next goals will be contacting these emitters by putting a gate structure on top of it, as well as creating single defects at higher wavelengths. [1] F. Hayee et.al., Nat.Mater.19 (2020) [2] C. Qian et.al., arXiv (2022)

MM 47.5 Wed 17:00 Poster B

Optimizing electrical transport and SAW propagation in molybdenum disulfide

— •Noah Spitzner[1], Pai Zhao[1], Renrong Liang[2], Chithra Sharma[1], Lars Tiemann[1], and Robert Blick[1] — [1]Center of Hybrid Nanostructures, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg — [2]School of Integrated Circuits, Tsinghua University, 100083 Beijing, China

Few-layered and monolayer MoS_2 has gained increasing significance in recent years, due to its large band gap of up to 1.9 eV at the K and K' valley of the hexagonal Brillouin zone. Surface acoustic waves (SAW) and transport measurements allow non destructive probing of the physics governing the material.

In this work we exfoliated MoS_2 flakes of a few layers onto a specially tailored substrate with $LiNbO_3$ as piezoelectric top layer. We can pass surface acoustic waves through the MoS_2 flake via an interdigitated transducer (IDT) electrode configuration and study the electrical response. To facilitate electron transport at low temperatures, liquid nitrogen physical vapor deposition (LNPVD) was utilized to deposit the contact metals. The cooled deposition reduces Fermi level pinning (FLP) in the contact interface and empowers us to measure longitudinal and transversal voltages with better contact quality.

Under acoustic excitation at 4.2 K, we observed acoustic currents and voltages in MoS_2 that depend on the power and frequency of the SAW. Hence, we were able to observe the acoustoelectric and acoustogalvanic effect. We also studied magnetotransport under perpendicular magnetic fields and the weak localization phenomenon.

MM 47.6 Wed 17:00 Poster B

Creating realistic carbon nanomembranes using molecular dynamics model simulations

— •Levin Mihlan[1], Anna Niggas[2], Filip Vukovic[2], Jürgen Schnack[1], and Richard A. Wilhelm[2] — [1]Universität Bielefeld, Deutschland — [2]TU Wien, Österreich

1nm thin carbon nanomembranes (CNMs) are synthesized from aromatic self-assembled monolayers (SAMs) by electron-induced crosslinking and supposedly of irregular internal structure, which renders standard spectroscopic characterization very difficult [1]. However MD simulations can offer insights into CNMs' internal structure. Recently, it was shown that the neutralisation dynamics of highly charged ions (HCIs) transmitting through thin materials are very sensitive to the material structure [2]. Hence, HCI spectroscopy may, together with accompanying simulations using a time dependent potential [3], be used to characterize CNMs. In order to obtain model membranes whose mechanical and spectral properties , fit to those of manufactured CNMs, a model process starting from a SAM is implemented as an MD simulation. Structures generated this way can be compared to alternative model structures, which are created by incorporating experimental mechanical properties as input parameters. This approach helps to gain a better understanding of the internal structure of CNMs.

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MM 47.7 Wed 17:00 Poster B

Rolle of Collective Behavior of Water Molecules in Robust Ferroelectricity in Graphene Nanoribbons

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An understanding of the water dynamics on the edges of one and two-dimensional structures is scarce. Still, such interactions can be sufficient to perturb local electric environments, therefore offering an opportunity to harness the effect of the local dipole moment of water. Combining experiments on nanoribbon field effect transistors and molecular dynamic simulations, we elucidate a collective behaviour of water within clusters adsorbed on graphene edges. We show that these nanoribbons exhibit significant and persistent remanent fields which can be employed in ferroelectric heterostructures and neuromorphic circuits.

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MM 47.8 Wed 17:00 Poster B

Experimental setup for gas sensing with TMD based field-effect devices

— •Axel Printschler[1], Emad Najafidehaghani[1], Antony George[1], Hamid Reza Rasouli[1], David Kaiser[1], Uwe Hübner[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena — [2]Leibniz Institute of Photonic Technology (IPHT), Jena

Sensing devices based on 2D transition metal dichalcogenides (TMDs) such as MoS_2, WS_2, $MoSe_2$, WSe_2, *etc.* have attracted significant research interest, as their electronic properties are greatly influenced by variations in the environment, *e.g.*, due to formation of adsorbates. This influence is reflected in changes of the device's electric transport characteristics, which can be precisely measured and used for gas sensing. As toxic gases pose a threat in many fields, there is a high demand in sensitive, selective and flexible gas sensors that also work at low power. Electronic sensors based on TMDs can satisfy this need while being atomically thin and flexible. Here we present an experimental setup and first results on gas sensing with field effect transistors (FETs) fabricated from TMD monolayers grown by chemical vapor deposition (CVD).

MM 47.9 Wed 17:00 Poster B

MOCVD synthesis of MoS2 and WS2 combination 2D heterostructures

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Two-dimensional (2D) materials (such as MoS2 and WS2) are materials layered at the atomic scale. This gives them exceptional electrical, mechanical and optical properties, and makes them interesting for electronics, photovoltaics and sensing [1]. Van der Waals heterostructures composed of 2D materials expand on the possible range of properties and so have attracted extensive focus due to factors such as smooth heterostructure interfaces, ultrafast carrier transport, and high bandgap tunability [2].

Here we present the synthesis of MoS2/WS2 combination heterostructures via metal-organic chemical vapour deposition (MOCVD) using a high controllable industrial scale multi-precursor system, and show the clearly defined stacked nature of the films produced. We explore the growth parameter space using Raman and X-ray photoemission spectroscopy, and microscopy techniques. We complement our characterisation by examining the influences on the band structure of the layered material.

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[2] W. Xia et al., Nanoscale 9, 4324-4365 (2017)

MM 47.10 Wed 17:00 Poster B

RF-sputtering of Nb and NbN thin films for quantum transport studies

— •Peer Heydolph, Vincent Strenzke, Isa Moch, Annika Weber, Lars Tiemann, and Robert Blick — Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Niobium plays a vital role in research and applications, contributing to advancements in superconductivity, quantum computing, and high-performance electronics. Here, we investigate the impact and interdependence of growth parameters on the properties of radio-frequency (RF)-sputtered niobium (Nb) and niobium nitride (NbN) thin films with a high critical temperature for applications in nanostructures and quantum transport studies at 4.2 Kelvin. We demonstrate that high quality superconducting films can be consistently produced even in a basic sputtering setup. We systematically varied the growth parameters such as the power of the RF-plasma and the flow of argon and nitrogen and survey their effects and interdependence on the properties of the thin films. The quality of the resulting films was characterized via X-ray diffraction (XRD), scanning electron microscopy (SEM) and profilometer measurements to gauge the film thickness. For electrical characterization at various temperatures and magnetic fields we employed a PPMS cryostat. We found that lower flow rates or RF powers do not necessarily lead to a higher critical temperature for NbN, which is in agreement with previous publications. Furthermore, it is crucial to finely tune all parameters and take into account their interdependencies.

MM 47.11 Wed 17:00 Poster B

Poly(neutral red) as a Possible Electrode Material for Electrochemical Cells

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Poly(neutral red) (PNR) is used in sensors owing to its redox characteristics and high electrical conductivity. PNR is also easy to prepare and inexpensive. Therefore, it might also be of interest as an electrode material in electrochemical cells like, e.g., electrochromic cells, batteries, or dye-sensitized solar cells (DSSCs). In the latter case, it could even help to replace platinum as an electrode material, which is expensive and not readily available. In this study, thin films of PNR were prepared by an established electrosynthetic procedure by oxidation of neutral red by cyclic voltammetry (CV) in an aqueous solution.[1] Samples were produced for varied number of oxidative cycles and then analysed for their layer thickness and absorptance. As expected, the layer thickness increased linearly with the number of cycles, as did the absorptance. The reversible electrochemical reduction and reoxidation of aqueous solutions of ferro/ferricyanide in contact to the prepared films was studied as a model electrolyte. Results and implications for the applicability of such PNR electrodes will be discussed. [1]. Y. Harada, D. Kono, P. Stadler, T. Yoshida, SPAST Abstracts ,1(01), First International Conference on Technologies for Smart Green Connected Society 2021.

MM 47.12 Wed 17:00 Poster B

Growth of Sc(x)Ga(1-x)N on 6H-SiC by plasma assisted molecular beam epitaxy

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ScGaN can occur in various crystal orientations. The most important are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition can be found between these orientations. Plasma-assisted molecular beam epitaxy (PAMBE) in combination with reflective high-energy electron diffraction (RHEED) was performed to create layers with different scandium concentrations in ScGaN. To determine the concentration of the grown layers, X-ray photoelectron spectroscopy was used in the same vacuum chamber. In addition, the surfaces were analyzed using atomic force microscopy (AFM, in-situ) and scanning electron microscopy (SEM) to obtain information on the morphology of the surfaces and to confirm the gained crystal orientations X-ray diffraction (XRD) were performed.

MM 47.13 Wed 17:00 Poster B

Optical and morphological properties of thin Nb2O5 layers deposited via High Power Impulse Magnetron Sputtering

— •Christof Zickenheiner[1], Raul Ramos[2], Viktor Udachin[1], Wolfgang Maus-Friedrichs[1], and José R.R. Bortoleto[2] — [1]Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [2]Instituto de Ciencia e Tecnologia, Sorocaba, Brazil

To address climate challenges and sustainable development, the UN set ambitious goals. Renewable energy, particularly solar, plays a key role. Emerging technologies like perovskite solar cells (PSC) offer cost-effective production, competing with silicon-based counterparts. This study focuses on the electron transport layer in PSC using Nb_2O_5 thin films deposited on glass substrates via HiPIMS from an Nb-target in an Ar/O_2 atmosphere at 25 °C. Pulse duration and oxygen pressure were varied as experimental parameters. Optical emission spectroscopy (OES) revealed the presence of oxygen species within a plasma and excitation of sputtered metal species for the HiPIMS process. The examination of the morphological properties via profilometry and contact angle analysis showed an influence of the experimental parameters on roughness. That is, shorter pulses as well as lower oxygen pressure result in smoother layer growth with a lower deposition rate. The investigation of optical properties via UV/Vis-Spectroscopy showed no significant impact of pulse duration. It became evident that lower oxygen pressure reduces the incorporation of oxygen into the growing layer. This results in a changed phase composition, with the formation of NbO_2, which in turn affects optical and electrical properties.

MM 47.14 Wed 17:00 Poster B

An attempt to predict oligomer sputtering using binary collision approximation simulations

— •Hans Hofsäss, Felix Junge, and Patrick Kirscht — II. Physikalisches Institut, Universität Göttingen, Germany

The binary collision approximation (BCA) program IMINTDYN [1] allows a prediction of ion solid interactions. For sputtering of carbon and SiO2 experimental sputter yields are significantly higher than yields from BCA simulations. SDTrimSP simulations [2] reproduce experimental sputter yields by adjusting the surface binding energies. For O atoms 1 eV instead of the elemental sublimation energy of 2.58 eV and for carbon 4.5 eV instead of 7.4 eV is used. For sputtering of carbon it was shown [3] that sputtering of oligomers and clusters is relevant. We introduce a model to simulate oligomer sputtering using the IMINTDYN program based solely on thermodynamic formation enthalpies. In particular sputtering of O2 and SiO dimers and carbon oligomers is energetically favorable. To predict the oligomer sputter fraction, we use Boltzmann factors based on the ratios of oligomer and monomer formation enthalpies. We show that we can quantitatively predict the carbon and SiO2 experimental sputter yields.

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MM 47.15 Wed 17:00 Poster B

Growth of Antimony thin films on c-plane Sapphire

— •Jonathan Spelsberg, Alexander Fuhrich, and Martin Salinga — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Antimony has been demonstrated to function as a single-element phase change material for electronic memory applications [1]. Confinement into nanostructures is crucial for stabilizing the amorphous phase of this material that is otherwise known for its fast crystallization kinetics. Yet, the exact influence of interfacing dielectrics on the physical properties of Antimony requires a fundamental investigation. To this end, samples with a well-controlled interface are required. Here, we report about the growth of Antimony thin films on c-plane Sapphire by molecular beam epitaxy. Based on characterization with RHEED and AFM, we demonstrate the impact of substrate preparation and process temperatures on the growth of 3 nm to 30 nm thick antimony films. Moreover, we discuss the relevance of Antimony cluster size and the effective use of a cracker effusion cell.

[1] M.Salinga et al., Monatomic phase change memory, Nature Materials 17, p. 681-685 (2018)

MM 47.16 Wed 17:00 Poster B

Novel nanofabrication facility for ultra-clean samples

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We present the capabilities of a novel nanofabrication facility dedicated

to the fabrication of nanostructures under ultra-clean conditions. In addition to a UHV cluster for MBE growth, the system comprises a lithography unit in an inert argon atmosphere. Air- and water-sensitive samples, like materials for memristive switches, can be structured using thermal scanning probe lithography with a lateral resolution down to less than 30 nm. Samples can be analyzed in-situ using RT-STM and RHEED. A self-sufficient UHV suitcase is used to characterize samples in other setups, such as femtosecond-laser pump probe spectroscopy, without ever exposing our samples to air.

MM 47.17 Wed 17:00 Poster B

Preparation and Characterization of Mixed Electrodes of WO_3 and MoO_3 as Electrochromic Coatings — •Smail Mekhilef, Thi Hai Quyen Nguyen, and Derck Schlettwein — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen

Electrochromic coatings can modify the transmittance for ambient light. As smart windows for buildings, relevant contributions can be expected for the energy-efficiency of buildings. Sputter- deposited WO_3 is typically used. Sustainability can be increased if low-temperature processes are established that would, further, allow the use of low-impact and low-weight polymer substrates. For large-scale applications, one may want to avoid W as a critical element and, at least partly, replace it by more abundant Mo. In this study, we extended established wet-chemical methods to prepare porous thin film electrodes of WO_3 [1] towards the processing of mixed oxides of W and Mo. Thin films of different W/Mo were prepared and characterized by scanning electron microscopy, atomic force microscopy and, mainly, by spectroelectrochemical measurements in contact to an inert organic electrolyte at either constant or swept electrode potential and the results will be discussed. [1]. T. H. Q. Nguyen, F. Eberheim, S. Göbel, P. Cop, M. Eckert, T. P. Schneider, L. Gümbel, B. M. Smarsly, D. Schlettwein, Enhancing the Spectroelectrochemical Performance of WO_3 Films by Use of Structure-Directing Agents during Film Growth, Appl. Sci. 2022, 12, 2327.

MM 47.18 Wed 17:00 Poster B

Deposition of reduced ceria thin films by reactive magnetron sputtering for the development of a resistive gas sensor — •Paul-G. Nitsch[1], Markus Ratzke[1], Emilia Pozarowska[2], Jan I. Flege[2], Carlos Alvarado Chavarin[3], Christian Wenger[3], and Inga A. Fischer[1] — [1]Experimentalphysik und funktionale Materialien, BTU-CS, Cottbus, Germany — [2]Angewandte Physik und Halbleiterspektroskopie, BTU-CS, Cottbus, Germany — [3]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany

The use of cerium oxide for hydrogen sensing is limited by the low electrical conductivity of layers deposited from a ceria target. To increase the electrical conductivity, partially reduced cerium oxide layers were obtained from a metallic cerium target by reactive magnetron sputtering. The proportions of the oxidation states Ce3+, present in reduced species, and Ce4+, present in fully oxidized species, were determined by ex-situ XPS. For electrical characterization, films were deposited on planarized tungsten finger electrodes. IV curves were measured over several days to investigate possible influences of oxygen and humidity on electrical conductivity. The morphological stability of the layers under ambient conditions was investigated by microscopical methods. The XPS results show a significant amount of Ce3+ in the layers. The electrical conductivity of as-grown samples is several orders of magnitude higher than that of samples grown from a ceria target. However, the conductivity decreases over time, indicating an oxidation of the layers. The surface morphology of the samples was found to be changing drastically within days, leading to partial delamination.

MM 47.19 Wed 17:00 Poster B

Modification of the optical and electrical properties of AZO thin films for variety of applications — •Maria Stefanova[1], Dimitrina Petrova[1,2], Blagovest Napoleonov[1], Stefani Bogoeva[1], Vladimira Videva[1,3], Velichka Strijkova[1], Vera Marinova[1], and Dimitre Dimitrov[1,4] — [1]Institute of Optical Materials and Technologies-BAS Sofia, Bulgaria — [2]South-West University "Neofit Rilski", Blagoevgrad, Bulgaria — [3]Sofia University, Sofia, Bulgaria — [4]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Here we report on the deposition of Aluminium Doped Zinc Oxide (AZO) thin films on sapphire substrates (AZO/Sapphire) by using ALD method and the influence of postdeposition UV-Ozone treatment on the films' properties. XRD revealed a polycrystalline wurtzite structure. The influence of UV-Ozone treatment on surface morphology, electrical and optical properties of AZO/Sapphire was investigated. It was found that UV-Ozone treatment improves the electrical and optical properties while did not cause significant changes to the polycrystalline structure and surface morphology of the AZO films which opens potential for various practical applications.

Acknowledgements This work is supported by the Bulgarian National Science Fund under the grant number KP-06-N-68/1 and the Research equipment of distributed research infrastructure INFRAMAT (part of Bulgarian National roadmap for research infrastructures) supported by Bulgarian Ministry of Education and Science.

MM 47.20 Wed 17:00 Poster B

Transient Photoluminescence of Lead Halide Perovskites Beyond Lifetimes: Non-excitonic Geminate Pairs and Carrier Transport — •Hannes Hempel[1], Martin Stolterfoht[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin, Germany — [2]Chinese University of Hong Kong, China

Transient photoluminescence (trPL) is the standard technique to quantify the lifetimes of photogenerated charge carriers in energy conversion materials. However, trPL decays are sensitive to processes other than only carrier recombination. We show that the initial trPL transients of lead halide perovskite thin films on glass are dominated by charge transport, namely hot carrier transport, spread-out of non-excitonic gemmate pairs, and redistribution. Including these processes in the modeling of trPL yields the doping and intrinsic carrier concentration, the mobility and diffusion coefficient, the hot carrier transport length, and the radiative and non-radiative lifetimes. Further, we calibrate trPL to absolute photon numbers, which allows quantifying the transient quasi-Fermi-level splitting and reveals fundamental energy losses in photo absorbers such as the increase of entropy by loss of geminate correlation and redistribution. The presented analysis is crucial for the appropriate interpretation of trPL and yields almost all optoelectronic properties relevant for application as a photo-absorber in solar cells.

MM 47.21 Wed 17:00 Poster B

Ultrafast Lattice Dynamics in Epitaxially Grown Bismuth Thin Films — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], Abdur Rehman Jalil[3], Julian Mertens[1], and Matthias Wuttig[1,2,3] — [1]I.Institute of Physics (IA) RWTH Aachen University — [2]Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]PGI 10 (Green IT), Forschungszentrum Jülich GmbH

Femtosecond optical pump probe measurements are carried out in order to detect changes in the reflectivity of the material response of epitaxially grown bismuth thin films on sub-ps timescales. Examination of reflectivity changes due to the coherent phonon response provides insight into the ultrafast lattice dynamics and relaxation of bismuth thin films. The pronounced thickness dependent behavior of bismuth is analysed by coherent phonons within the framework of displacive and impulsive excitation models. Here, we show how the competition of phonon softening due to different laser fluencies and phonon hardening from confinement effects can be understood. Raman measurements are carried out to help to disentangle both effects. XRD measurements are shown to help to understand the structural change of the lattice structure. These combined measurements will help to understand confinement and fluency effects in a single model and shows how to tune bonding properties in this unconventional class of materials.

MM 47.22 Wed 17:00 Poster B

Atomic-Scale Insights Into The Interlayer Characteristics of Thin-Layered Materials Using Ultra-high Vacuum Tip-Enhanced Raman Spectroscopy — •Soumyajit Rajak and Nan Jiang — University of Illinois Chicago, Chicago, USA

Optoelectronic properties of molecular thin films are controlled by the local nanostructures of a molecular arrangement. Probing the effect of the local environment of nanostructures is challenging because the spatial resolution of conventional optical spectroscopic techniques is limited by the diffraction limit of light. Coupling light with plasmonic nano-objects creates highly localized surface plasmons (LSPs), which allows us to break the diffraction limit. Herein we present a combined topographical and optical analysis of different surface-sensitive arrangements of molecules and 2D material heterostructures using angstrom-scale resolution scanning tunneling microscopy (STM) and ultra-high vacuum tip-enhanced Raman spectroscopy (UHV-TERS). TERS uses the apex of an STM tip made of a plasmonic metal to couple light to the near field. The Raman modes of the nanostructure underneath this tip are enhanced by the nano-confined surface plasmons which allows us to obtain chemical information with Angstrom scale spatial resolution. STM images combined with localized surface plasmon resonance-enhanced Raman signals reveal different adsorbate configurations of single molecule entities and a fundamental view of interfacial interactions. The atomic scale insights obtained into the local environment enable precise control over the fabrication of nanostructures with tailored optoelectronic properties.

MM 47.23 Wed 17:00 Poster B

In-situ Study of Surface Band-Bending in c-ZnO and its Effect on the Excitonic Dielectric Function — •Luis Rosillo Orozco[1], Kurt Hingerl[1], and Christoph Cobet[1,2] — [1]Zentrum für Oberflächen und Nanoanalytik, Johannes Kepler Universität, Linz, Austria — [2]Linz School of Education, Johannes Kepler Universität, Linz, Austria

Semiconductors in air and in vacuum often have a band-bending near the surface caused by surface states capturing bulk charges or simply due to natural polarization in the case of polar materials, as is the case of Zinc Oxide. Nevertheless, when semiconductors are in contact with an electrolyte we can intentionally produce a surface dipole and create a space charge region (SCR) by adding another electrode in the solution and applying a voltage between the two.

Space charge regions have a big impact on the optical and electrical properties of semiconductors and, of course, semiconductor devices. Therefore, it is of high interest to understand the effects caused by them.

We present in-situ spectroscopic ellipsometry (SE) combined with electrochemical techniques to study the response of the discrete excitons and exciton-phonon complexes (EPC) to the inner electric fields produced near the semiconductor surface. Using mono-chromatic transients we are able to identify the flat-band potential. A semi-empirical optical model is developed to study the contribution of the surface band-bending to the total dielectic function for a range between 3.2 e.V. to 3.6 e.V.

MM 47.24 Wed 17:00 Poster B

In situ optical tracking of oxidation state changes of NiFe alloys by Reflectance Anisotropy Spectroscopy — •Sandhya Chandola[1], Karuppasamy Dharmaraj[2], Jörg Rappich[1], Norbert Esser[3,4], and Sonya Calnan[2] — [1]Young Investigator Group Nanoscale Solid-Liquid Interfaces (CE-NSLI), Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Kompetenzzentrum Photovoltaik Berlin, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [4]Leibniz-Institut für Analytische Wissenschaften ISAS e.V., Schwarzschildstr. 8, 12489 Berlin, Germany

The oxygen evolution reaction (OER) is a key reaction involved in water splitting and has attracted increasing attention for hydrogen generation for clean energy uses. Nickel/iron (NiFe)-based compounds have been known as active OER catalysts for decades, and there has been increasing interest in developing NiFe-based materials for higher activity and stability.

Reflection Anisotropy Spectroscopy (RAS) in the visible spectral range is a polarisation sensitive optical spectroscopy technique used to study morphological and electronic structure changes of surfaces and thin films in-situ. It achieves high sensitivities in the detection of ultrathin layer structures down to the sub-nanometer scale and can follow the optical changes of the surface during catalytic reactions. By combining in-situ RAS and cyclic voltammetry (CV), the changes in both the redox state and structural phase during OER activity of NiFe alloys can be optically tracked.

MM 47.25 Wed 17:00 Poster B

Triptycene as a versatile building block for self-assembled monolayers — Takanori Fukushima[1], Manfred Buck[2], Egbert Zojer[3], and •Michael Zharnikov[4] — [1]Tokyo Institute of Technology, Yokohama 226-8503, Japan — [2]EaStCHEM School of Chemistry, University of St Andrews, St Andrews KY16 9ST, UK — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria — [4]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

When employing self-assembled monolayers (SAMs) for tuning surface- and interface-properties, a strong binding to the substrate, structural uniformity, and the ability to align functional groups and to control their density are desirable. To achieve these goals, tripod systems bearing multiple bonding sites have been developed as an alternative to conventional monodentate systems. A bonding of all three sites has, however, hardly been achieved with the consequence that structural uniformity and orientational order in tripodal SAMs are usually quite poor. To resolve that problem, we designed a series of triptycene-based molecules decorated with three anchoring groups, which can be assembled on different substrates. Depending on the character of the anchoring groups, well-defined tripodal SAMs could be prepared on Au(111), Ag(111), and indium tin oxide. Either unsubstituted or differently substituted triptycene-based molecules were assembled in context of different issues, viz. (i) homogeneous tripodal assembly, (ii) polymorphism and hidden chirality, (iii) on-surface click chemistry, (iv) multiple pathways in charge transfer, and (v) nanofabrication.

MM 47.26 Wed 17:00 Poster B

A new design concept for SAMs of N-heterocyclic carbenes — Mateusz Wróbel[1], Daria M. Cegiełka[1], Andika Asyuda[2], Krzysztof Kozieł[3], •Michael Zharnikov[2], and Piotr Cyganik[1] — [1]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [3]Faculty of Chemistry, Jagiellonian University, 30-387 Krakow, Poland

Self-assembled monolayers (SAMs) of N-heterocyclic carbenes (NHCs) on metal substrates are currently one of the most promising systems in context of molecular engineering of surfaces and interfaces. Interest in these systems is mainly driven by their assumingly higher thermal stability compared to thiolate SAMs most broadly used at the moment. Most of the NHC SAMs utilize imidazolium as an anchoring group for linking molecules to the metal substrate via carbene C atom. It is well established in the literature that upright-oriented and stable NHC SAMs can only be built when using bulky side groups attached to nitrogen heteroatoms in imidazolium moiety, which, however, reduce significantly the packing density. In contrast, combining several complementary experimental techniques, we show that aromatic monolayers exhibiting at least double surface density, upright molecular orientation, and ultra-high thermal stability compared to the NHC SAMs reported before can be readily fabricated on the basis of NHCs with small methyl side groups in combination with simple solution-based preparation procedure. These parameters are crucial for numerous applications, including molecular and organic electronics.

MM 47.27 Wed 17:00 Poster B

Interaction study between thin films of polyvinyl acetate and (plasma-treated) aluminum — •Sascha Zimmermann[1], Philipp Moritz[1], Oliver Höfft[1], Lienhard Wegewitz[1], Wolfgang Maus-Friedrichs[1], and Sebastian Dahle[2] — [1]Clausthal University of Technology, Germany — [2]University of Ljubljana, Slovenia

Composite materials made of wood and aluminum are becoming increasingly popular due to the combination of their properties. However, in order to exploit these advantages, the two materials must be bonded with sufficient stability. While the adhesive polyvinyl acetate (PVAc) exhibits high adhesive strength on wood, its bonding capabilities with aluminum are limited. The surface of the aluminum must therefore be modified. In this work, the aluminum surface is treated with a dielectric barrier discharge plasma in air with the aim of enabling molecular interactions. Various analytical techniques, including X-ray photoelectron spectroscopy (XPS), Reflection Absorption Infra-Red Spectroscopy (RAIRS) and Atomic Force Microscopy (AFM), are employed to analyse the chemical interactions between aluminum and PVAc. This involves producing nm-thin films using spin coating. For untreated aluminum, no interactions were detected. AFM revealed the inability to deposit nanometer-thin films due to the lack of interactions, leading to the formation of PVAC-clusters. Plasma-treated aluminum led to a stronger chemical shift in the XPS spectra indicating hydrogen bonding. This finding was confirmed by RAIRS, which shows bands associated with hydrogen bonding.

MM 47.28 Wed 17:00 Poster B

Spectroscopical properties investigation of pyrene based molecules in perspective of singlet fission — •Sruthy Asa Rajan, Sergey Bagnich, and Anna Köhler — Universität Bayreuth, Bayreuth, Germany

Photovoltaics plays a vital role in renewable energy. Theoretically, convectional silicon solar cells' efficiency is limited to 33% known as the Shockley-Queisser limit, which is limited by some practical and fundamental losses like thermalisation loss. Singlet fission (SF) is a carrier multiplication process, which has the potential to overcome Shockley-Queisser limit. In an organic semiconductor, chromophore in its singlet excited state shares its energy with a nearby ground-state chromophore to form two triplet excitons. Recent studies shown that some pyrene derivatives exhibit SF. A study has shown that bridged SF chromophore forms generated triplet pair and hence leading to formation of long-lived triplets.

We are investigating the impact on absorption, photo-luminescence, lifetime decay, time-resolved spectroscopy and quantum yield of different N-substitution groups on para Diketopyrrollopyrrole (PDPP) based pyrene derivatives, which have a comparable triplet energy to silicon bandgap. We will focus more on the changes in morphology of film of these compounds by varying the conditions of film preparation, such solvents, annealing effect, etc. We hypothesis that certain orientation of these pyrene-base molecules can trigger singlet fission.

MM 47.29 Wed 17:00 Poster B

Understanding the disparate interactions of thin polymer films with natively oxidized metal surfaces and metal oxide crystals — •Friedrich Bürger, Philipp Moritz, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

In the Collaborative Research Centre 1368 “oxygen free production” the molecular interactions between thin films of commonly used polymers, poly(ethyl cyanoacrylate) (PECA) and poly(methyl methacrylate) (PMMA), and different metal oxides have been characterized. In the context of this project, certain interactions became apparent, e. g. hydrogen bonding or ionic interactions that were observed on natively oxidized samples representing very thin oxide films. In contrast, these interactions were absent on a TiO_2 single crystal. To investigate if this effect is reproducible and inherent to metal oxide single crystals, the interactions of PECA and different metal oxide single crystals are determined using X-Ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS) and Metastable Induced Electron Spectroscopy (MIES). These results are compared to the interactions of natively oxidized metal samples with thin polymer films. Assuming reproducibility, a root cause for the disparate interactions is proposed.

MM 47.30 Wed 17:00 Poster B

Influence of processing atmospheres on curing and bonding of cyanoacrylate adhesives — •Philipp Moritz, Oliver Höfft, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Technical University Clausthal, Clausthal-Zellerfeld, Germany

Cyanoacrylates are fast-curing adhesives that are often used in joining technology to bond components together quickly. The curing and strength of the bond are often improved with numerous additives and surface pre-treatments. However, the surrounding process atmosphere is an aspect that has hardly been used to control curing and adhesive interactions.
To investigate the interactions and curing, thin films of cyanoacrylate are deposited on natively oxidized copper substrates. The surrounding atmosphere is varied between (i) air atmosphere, (ii) argon and (iii) an oxygen-free environment (O_2 partial pressure $< 10^{-20}$ mbar). The curing and underlying molecular interactions at the interface between cyanoacrylate and oxidized copper are investigated using spectroscopic and microscopic methods.
Curing in argon and the O_2-free atmosphere is significantly slower than in air. Nevertheless, strong interactions occur in an oxygen-free atmosphere and air, e.g. hydrogen bonds and ionic interactions. In argon, on the other hand, no molecular interactions are observed.
Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 394563137 – SFB 1368.

MM 47.31 Wed 17:00 Poster B

The influence of PDMS residues on the mobility of molecules deposited onto Si/SiO2 wafers — •Erik von der Oelsnitz[1,2], Tim Völzer[1,2], Julian Schröer[1], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]Institute of Physics, University of Rostock, Germany — [2]Department ”Life, Light & Matter”, University of Rostock, Germany

The exfoliation and stamping of flakes of 2D materials onto a substrate is one of the most used methods for the preparation of transition metal dichalcogenide (TMDC) monolayers. However, it was found that during the transfer of the flake, impurities and in particular residues of the common stamp material polydimethyl siloxane (PDMS) are transferred to the substrate. This could have a major impact when analyzing TMDCs, especially in TMDC/molecule hybrid structures. In order to examine the effect of these impurities, dye molecules were evaporated onto a Si/SiO2 wafer and then measured in a fluorescence lifetime microscope (FLIM). Here, in a certain area, the dye coverage is removed by laser-induced photodegradation and the diffusion of the molecules into this depleted area is examined. Three wafers are compared, each representing a specific step of the preparation process. The FLIM measurements showed that the molecules on the bare wafer diffuse into the depleted area the fastest, while they take significantly longer on the samples that came into contact with PDMS. This shows that the surface properties of exfoliated 2D materials are significantly influenced by the contact with PDMS, which in turn has a major effect on the mobility and thus the dynamics of deposited molecules.

MM 48: Members’ Assembly

Time: Wednesday 18:30–21:00 Location: H 0110

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 including our MM get-together for personal exchange.

MM 49: Invited Talk: Daniel Sopu

Time: Thursday 9:30–10:00 Location: C 130

Invited Talk MM 49.1 Thu 9:30 C 130

STZ-vortex unit, a step forward in understanding and controlling shear banding in metallic glasses — •Daniel Sopu — Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria — Darmstadt University of Technology, Germany

The ability to control plastic deformation of metallic glasses is based on the capacity to influence the percolation of shear transformation zones (STZs) that ultimately leads to shear band formation. In this talk, using molecular dynamics and athermal quasi-static simulations, we propose a novel atomic-level mechanism underlying the STZ activation and percolation processes, which could provide a robust microscopic description of shear band formation and propagation in metallic glasses. The proposed mechanism entails two main units: large shear strains (i.e. STZs) and vortex-like (i.e. rotating) structures. Such a vortex-like flow corresponds to a strong rigid rotation of groups of atoms which, in turn, appears to be a necessary step to activate the subsequent STZ through a kind of autocatalytic process.

So far, STZ-vortex mechanism allowed to follow the structural and dynamical evolution during shearing in metallic glasses and provided an atomistic description of deformation mechanisms such as shear band formation and interaction, shear band branching and multiplication or shear band blocking and deflection. This new model can further contribute to the understanding and control of shear banding behavior and the avoidance of runaway instability, thereby improving the plastic deformability of metallic glasses.

MM 50: Focus Session: Battery Materials – Ion Transport, Impurity Effects and Modelling (joint session KFM/MM)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques , thermal characterisation techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Chair: Ilyas Mohsin (KIT Karlsruhe)

Time: Thursday 9:30–13:35 Location: EMH 225

Invited Talk MM 50.1 Thu 9:30 EMH 225

Ion transport in battery electrolytes and related interphases — •Jelena Popovic-Neuber — University of Stavanger, Norway

The development of next generation batteries depends heavily on the capability of electrolytes to quickly and selectively transport alkali and alkaline earth metal cations, and form stable electrochemical interfaces. In the first part of my talk, current understanding of ion transport mechanisms and related electrochemical measurement techniques (impedance spectroscopy, galvanostatic polarization) in soft matter battery electrolytes including liquids, polymers and hybrid materials will be discussed. According to this discussion, I will give guidelines and examples of improvements of the relevant electrochemical properties including ionic conductivity and the cationic transference number. In the second part of my talk, I will show recent findings related to the electrochemical and chemical growth and transport in SEIs on several alkali and alkaline earth metal anodes in contact with liquid and solid-state electrolytes. The multitechnique approach involving the measurement of activation energy for ion transport showed that such SEIs are complex composite liquid/solid materials, with sometimes predominant ionic pathways in the liquid phase. The relevance of the native passive layer on alkali and alkaline earth metals, possibility of forming artificial SEIs and electrodeposition through porous SEI will be discussed. Finally, I will show a new modelling approach for treatment of impedance spectroscopy data of symmetric alkaline and alkaline earth metal cells.

MM 50.2 Thu 10:00 EMH 225

NASICON as solid electrolyte for Mg- and Ca-ion batteries — •Katharina Helmrecht[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) for Electrochemical Energy Storage, Ulm, Germany

In Na-ion batteries, NASICON has been used as a solid-electrolyte material. Here we present a density functional theory study in which we investigate whether NASICON can also be a suitable solid electrolyte for bivalent charge carriers such as Mg and Ca. We have in particular chosen $Ca_{0.5}Ti_2(PO_4)_3$, $Ca_{0.5}Zr_2(PO_4)_3$, $Mg_{0.5}Sn_2(PO_4)_3$, and $Mg_{0.5}Zr_2(PO_4)_3$ for our investigation. We find that these phases indeed show promise as solid electrolytes.

Unlike the classic NASICON phase, which often undergoes a phase transition from rhombohedral to monoclinic within the battery's operating range, this issue does not arise with Ca and Mg. However, only half of the sites occupied by Na (specifically, the Na1 sites) become occupied by the bivalent carriers. We investigate the energetic ordering of the occupied positions inside and the diffusion mechanism inside the phase as well as bottleneck sizes and compare this to the classic NASICON phase.

MM 50.3 Thu 10:20 EMH 225

Rhombohedral (R-3) Prussian white cathode material: An ab-initio study — •Sebastian Baumgart[1], Mohsen Sotoudeh[1], and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) for Electrochemical Energy Storage, Ulm, Germany

The demand for efficient and sustainable cathode materials for alternative battery chemistries is ever more increasing. Prussian Blue analogues (PBAs) exhibit a long cycling life and a high rate capability, which makes them a promising cathode material for next-generation battery technologies. Notably, Prussian White (PW) exhibits a phase transition at high sodium and low vacancy content, transitioning to a rhombohedral (R-3) phase.

However, the detailed exploration of the rhombohedral modification and its electronic structure remains incomplete. In this study, we provide insights into why the rhombohedral structure manifests itself only at high sodium contents, employing atomistic first-principles calculations.

Our findings reveal the stabilization of the rhombohedral structure by sodium atoms. Additionally, we elucidate the changes in the sodium ion minimum energy position during the phase transition and analyze the sodium migration barrier within the cubic and rhombohedral phases, offering a comprehensive theoretical assessment of its viability as a battery material.

MM 50.4 Thu 10:40 EMH 225

Advancing Post-Lithium Batteries: Insights into Cathode Material Design and Electrochemical Stability — •Mohsen Sotoudeh[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Oberberghof 7, 89081 Ulm — [2]Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm

In the search for sustainable alternatives to the prevailing Li-ion batteries, key features that influence the activation energy barrier and electrochemical stability are investigated using periodic density functional theory calculations. The study employs a novel descriptor to determine the ionic mobility and highlights the critical role of ionic radii, oxidation state, and electronegativity on the mobility as well as the stability of crystalline materials, providing practical guidelines for the selection of promising solid materials. At the same time, the potential of Mg batteries with oxide cathodes is explored, recognizing the challenges posed by the sluggish kinetics of Mg^{2+} migration. Promising candidates, guided by theoretical insights, have been synthesized and structurally characterized, paving the way for the exploitation of functional cathode materials with improved Mg^{2+} transport properties. In addition, the electrochemical stability of binary and ternary spinel compounds is investigated, with potential applications as protective coatings, and solid electrolytes in batteries. This comprehensive study provides critical insights into the development of new battery technology for high-performance energy storage solutions.

The work has been supported by the DFG through Excellence Cluster EXC-2154, project No. 422053626.

MM 50.5 Thu 11:00 EMH 225

Remodeling interfacial electrical field for superhigh capacity and ultralong lifespan aqueous zinc-ion batteries — •Yan Ran[1], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

Herein, density functional theory (DFT) calculations studied the NH4V4O10@carbon cloth (NVO@CC) as a high-performance cathode material at the heterostructure interface for AZIBs. The electronic structure, adsorption energy, and migration energy barrier prove there are additional active sites at the interface due to the built-in electric field between NVO and CC, which improves the conductivity and stability of the NVO@CC electrode material. Accordingly, the designed binder-free NVO@CC cathode exhibits high specific capacity (607.1 mAh/g at 0.1 A/g), an outstanding energy density (443.6 Wh/kg at 0.3 A/g), and an excellent long-term cyclability (the capacity retention rate is 81.24% after 10,000 ultra-long cycles at 5 A/g). This excellent electrochemical performance is attributed to enhanced conductivity and fast electrochemical kinetics by a series of ex-situ characterizations. This work reveals a binder-free self-grown flexible cathode on carbon cloth, which is promising for high-performance aqueous zinc ion batteries.

15 min. break

MM 50.6 Thu 11:35 EMH 225

Computational Screening of Chloride Perovskites as Cl^--Ion Solid Electrolyte — •Johannes Döhn[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Helmholtz Institute Ulm, Germany

The intermittency of wind and solar power - the solely sustainable energy sources which are considered to be abundantly available - leaves only one consequence: For the transition towards renewable energy systems, efficient and reliable storage technologies are needed. Batteries are one of the most widely used storage devices but current technology based on the transfer of Li-ions faces several challenges including their dependence on critical materials with respect to both, scarcity and toxicity.

In our contribution, we will present atomic-scale investigations of potential future battery materials carried out using density functional theory (DFT). We employed a high-throughput approach in order to screen the well known materials' class of chloride perovskites as solid electrolyte material for chloride ion batteries and we derived several properties as electrochemical stability and diffusion barrier for in total 148 compounds. Our screening focusses on the highly symmetric cubic perovskite structure but for the most promising candidates also the less symmetric distorted phases are investigated, additionally shedding some light on potential property-structure relationships.

Such in silico investigations significantly narrow down the potential materials space for our experimental coworkers and, thereby, contribute to finding green, cheap and reliable devices for energy storage.

MM 50.7 Thu 11:55 EMH 225

The role of the SEI for lithium whiskers in lithium metal batteries — •Martin Werres[1,2], Arnulf Latz[1,2,3], and Birger Horstmann[1,2,3] — [1]Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Ulm, Deutschland — [2]Helmholtz Institut Ulm (HIU), Ulm, Deutschland — [3]Universität Ulm, Ulm, Deutschland

Lithium metal (Li) batteries are promising due to their high specific energy. However, safety concerns and non-optimal cycle stability hold back Li anodes paired with liquid electrolytes.[1] A major challenge is the growth of Li whiskers. Li whiskers come with cycling inefficiencies, e.g., enhanced formation of isolated Li.[2] Understanding why Li whiskers emerge can help find design rules for safer Li batteries. We study plating/stripping of Li under the aspect of the mechanical properties of Li and the role of the covering solid-electrolyte interphase (SEI).[3] We consider a Li nucleus covered by SEI, which grows continuously during plating. Once the stress in the SEI exceeds a threshold, the SEI breaks. Due to the softness of Li and significant creep under the expected stress conditions, Li can extrude through the hole in the SEI. We model this by approximating Li as a Herschel-Bulkley liquid. Our predicted shapes and growth rates are consistent with the experimental observation of Li whiskers. We deduce that the SEI is the most important design parameter to achieve safe Li batteries.

[1] B. Horstmann et al., Energy Environ. Sci. 2021, 14(10), 5289-5314. [2] M. Werres et al., ACS Nano 2023, 17(11), 10218-10228. [3] L. von Kolzenberg et al., Phys. Chem. Chem. Phys. 2022, 24(31), 18469-18476.

MM 50.8 Thu 12:15 EMH 225

Elucidating the Silicon Voltage Hysteresis by Mechanical Coupling of Anode Particles and SEI — •Lukas Köbbing[1,2], Arnulf Latz[1,2,3], and Birger Horstmann[1,2,3] — [1]German Aerospace Center (DLR), Ulm, Germany — [2]Helmholtz Institute Ulm (HIU), Ulm, Germany — [3]Ulm University, Ulm, Germany

Silicon promises to be a superior next-generation anode material. However, a major challenge of silicon anodes is the significant voltage hysteresis reducing efficiency and leading to detrimental heat generation. Additionally, the hysteresis hinders precise state-of-charge estimation. Our recent research identifies the chemo-mechanical coupling of silicon and the Solid-Electrolyte Interphase (SEI) as the reason for the substantial voltage hysteresis. The SEI is a thin passivating film that grows on negative electrode particles due to electrolyte decomposition [1]. For silicon particles, volume changes lead to significant strains and plastic deformation within the SEI [2]. As anode particle and SEI are mechanically coupled, the stress generated inside the SEI impacts the stress inside the anode, affecting its potential. Our chemo-mechanical model reproduces the observed open-circuit voltage hysteresis [3]. Furthermore, our visco-elastoplastic SEI model reproduces the voltage difference between slow cycling and the relaxed voltage. This detailed physical understanding can improve the performance of silicon anodes. [1] L. Köbbing et al. J. Power Sources 2023, DOI: 10.1016/j.jpowsour.2023.232651. [2] L. Kolzenberg et al. Batter. Supercaps 2022, 5, DOI: 10.1002/batt.202100216. [3] L. Köbbing et al. Adv. Funct. Mater. 2023, DOI: 10.1002/adfm.202308818.

MM 50.9 Thu 12:35 EMH 225

Understanding SEI formation in Alkali Metal Batteries — •Daniel Stottmeister[1] and Axel Gross[1,2] — [1]Institut für Theoretische Chemie, Ulm University, Ulm, Germany — [2]Helmholtz Institute Ulm, Ulm, Germany

Batteries have established themselves as one of the prime energy storage devices in modern times. Due to the relative scarcity of lithium and the ever-increasing demand for safe, efficient, and affordable energy storage solutions, post-lithium battery systems have emerged as promising future energy storage solutions. Other more common alkali metals like sodium and potassium are of particular interest. However, like their lithium predecessors, sodium and potassium batteries suffer from various issues, some of which originate from the formation of an instable solid electrolyte interphase (SEI). The formation mechanisms of said SEI are yet to be fully understood. Density Functional Theory (DFT) is a well-established method for the description of systems at the atomic level and can help to unravel some of the reaction mechanisms relevant to the formation of the SEI. This contribution uses ab initio molecular dynamics (AIMD) and DFT simulations to investigate and compare the electrolyte decomposition and the resulting SEI formation mechanisms of lithium, sodium, and potassium metal batteries at the atomistic level.

MM 50.10 Thu 12:55 EMH 225

Effects of Aluminum trifluoride impurities on NMC811

/Graphite Lithium-ion battery performance. — •slaheddine Jabri — Institute of Applied Physics, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The effects of aluminum trifluoride (AlF3) impurities in the electrolyte of full cell lithium-ion batteries has been studied using NMC811/Graphite electrodes. A strong decline of the retention capacity is observed when the cells are cycled at 50 °C in the presence of AlF3 impurities in the electrolyte. The AlF3 accelerates the cell degradation by the generation of various compounds during battery operation. The NMC811 cathode and the Graphite anode are characterized with different techniques. Scanning electron microscopy SEM, including cross-section- Focus Ion Beam FIB, Raman spectroscopy and X-ray photoelectron spectroscopy XPS methods are employed to investigate the effect of the degradation on the electrolyte due to the AlF3 impurities. We found modified chemical components and morphology of the surface electrolyte interface (SEI) and cathode electrolyte interface (CEI) layers of anode and cathode after cell aging with polymer layers on the both surfaces. Pathways to understand the AlF3 impact are proposed.

MM 50.11 Thu 13:15 EMH 225

Impurity Effects of AlCl$_3$ on the Performance of Polyamide-Ionic-Liquid-based Polymer Electrolytes for Aluminium Batteries — •Mohammad Mostafizar Rahman, Amir Mohammad, Shuvrodev Biswas, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg

The AlCl$_3$-Et$_3$NHCl ionic liquid (IL) has emerged as a promising and cost-effective option for the rechargeable Al-ion battery system. The polyamide-based solid polymer electrolyte (SPE) derived from this IL was utilized for the present investigation. Six different purities of AlCl$_3$ salts (ranging from 98 % to 99.999 %) with variable prices were used to prepare the SPEs and their performance was evaluated using various electrochemical characterization techniques. The results indicate good reversibility and Al stripping/plating behavior without impurity effects. Conductivities range from 0.19 mS/cm to 0.21 mS/cm, while stability windows span 2.70 V to 2.83 V. In addition, specific capacities range from 28 mAh/g to 39 mAh/g with no systematic effect of impurities. Overall, the electrochemical analysis shows that impurities in AlCl$_3$ salts have minimal impact on the SPE electrochemical properties. A cost-benefit analysis indicates that utilizing a low-cost AlCl$_3$ salt (0.027 €/g) yields comparable electrolyte performance as a higher-priced (6.198 €/g) high-purity salt. This discovery enables a reduction in electrolyte cost by approximately a factor of 17, consequently leading to a decrease in the overall cost of Al batteries.

MM 51: Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides II (joint session DS/MM/O)

Surface functionalization & defects and Water & gas Interaction

Time: Thursday 9:30–12:15 Location: A 053

Invited Talk MM 51.1 Thu 9:30 A 053

Computational insights into the surface functionalization and defects in MXenes — •Hannu-Pekka Komsa — Microelectronics Research Unit, University of Oulu, Finland

Two-dimensional (2D) transition metal carbide and nitride MXenes offer rich chemistry with extraordinary properties. The surface of MXenes is terminated by -O, -OH, and -F groups during the synthesis. However, there is limited understanding on how the surface composition depends on the synthesis conditions and on the type of MXene (transition metal, carbon vs. nitrogen, and the number of atomic layers).

We developed a multi-scale computational scheme to simulate the distribution and the thermodynamically favorable composition of the functional groups on the MXene surfaces. We considered the most popular MXene systems such as Ti$_2$C, Ti$_3$C$_2$, Ti$_2$N, Ti$_4$N$_3$, Nb$_2$C, and Nb$_4$C$_3$. The surface accommodates mixtures of functional groups for all considered MXenes with similar distributions regardless of the type of metal, carbon or nitrogen species and number of atomic layers. These findings are shown to be important for an accurate prediction of properties and stability of these materials. Next, we investigated the propensity of metal vacancy formation under synthesis conditions. The results suggest that vacancy formation is crucial step in initiating MXene oxidation. Finally, to support experimental characterization, we simulated the Raman spectra as a function of functional group distribution, temperature, and disorder, and the materials' response to electron irradiation in electron microscope.

MM 51.2 Thu 10:00 A 053

In situ monitoring of surface termination of Ti3C2Tx MXene with Raman spectroscopy — •Julian Plaickner[1,2], Tristan Petit[2], Peer Bärmann[2], Thorsten Schultz[2,3], Norbert Koch[2,3], and Norbert Esser[1,4] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstrasse 36, 10623 Berlin — [2]Hardenbergstrasse 36 — [3]Institut für Physik & IRIS Adlershof, Humboldt Universität zu Berlin, 12489 Berlin — [4]Leibniz Institut für Analytische Wissenschaften ISAS eV, Schwarzschildstrasse 8, 12489 Berlin

In the last years, MXenes have attracted attention due to an interesting combination of physical properties. A better knowledge of the surface chemistry of MXenes is critical for the implementation in applications. A promising investigation approach is annealing-induced desorption of surface terminations, because it might make the surface very active for further functionalizations. In this work, the effect of annealing on the Ti3C2Tx MXene surface chemistry in UHV has been investigated with Raman spectroscopy in ultra-high vacuum. Changes in the Raman spectra are correlated with the desorption of the major part of the F surface termination at 650 °C. Most of the observed spectral features show a significant broadening already before annealing. We attribute this to the intrinsic disordered nature of the MXenes due to a mixed surface termination and a broad background associated to electronic Raman scattering. With this study we identified of the vibrational signatures associated with F-termination and provided new insights into the interpretation of the vibrational spectra of Ti3C2Tx MXenes.

MM 51.3 Thu 10:15 A 053

Hydrogenation as a mean to remove halogen functionalization from of Ti3C2Tz thin films — •Silvano Lizzit[1], Florian Brette[2,3], Hanna Pazniak[4], Monika Shied[1], Paolo Lacovig[1], Florent Boucher[3], Vincent Mauchamp[2], and Rosanna Larciprete[5] — [1]Elettra-Sincrotrone Trieste, Trieste (I) — [2]Uni. Poitiers, ISAE-ENSMA, CNRS, PPRIME, Poitiers (F) — [3]CNRS-IMN, Nantes (F) — [4]Uni. Grenoble Alpes, CNRS, Grenoble INP, Grenoble (F) — [5]CNR- ISC, Roma (I)

The nature and the density of the chemical groups terminating the MXenes surface determine their electronic and chemical properties. Therefore, the manipulation of the surface termination allows to change the way these compounds interact with the surrounding environment. In this study we explored the possibility of using the functionalization with H atoms as a mean to modify the surface termination of T3C2Tz thin films. To this aim we used photoelectron spectroscopy with synchrotron radiation to investigate the surface reactions induced by the exposure to atomic hydrogen. Simulation of the valence band spectra by DFT calculations combined with the analysis of the core level spectra allowed us to elucidate the changes in the chemical bonding determined by the interaction with H atoms. It turned out that, in addition to the formation of C-H and -O-H bonds, sample hydrogenation removed the halogen terminating atoms, decreasing the F and Cl concentrations to less than 20% of the initial values. After removing the hydrogenated phases at 400 K, the dehydrogenated surface exhibited a chemical reactivity higher than that of the pristine sample.

MM 51.4 Thu 10:30 A 053

Chemical characterization of defects in Ti3C2Tx MXenes by soft X-ray spectroscopy — •Arsène Chemin[1], Zoé Dessoliers[1], Robert W. Lord[2], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]A.J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, Pennsylvania, USA

MXenes offer a wide spectrum of properties with numerous fields of application. Yet, these properties can be strongly affected by defects, and a detailed understanding of their nature and structure is essential. Despite many observations of such defects, grasping their chemical natures is challenging. In this work, high-resolution X-ray Photoelectron Spectroscopy (HR-XPS) and, at the Ti L- and C,O K-edges, soft X-ray Absorption Spectroscopy (XAS), performed at the BESSY II synchrotron in Berlin, are used to investigate the chemical nature of defects in Ti3C2Tx MXenes.

15 min. break

Invited Talk MM 51.5 Thu 11:00 A 053

MXenes as materials for carbon capture, storage, and usage technologies: Computational insights & predictions — •Francesc Viñes — Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1-11, 08028 Barcelona, Spain

Environmentally-wise, pristine MXenes have been proposed as suited materials for carbon capture and storage (CCS) technologies, as predicted by computational density functional theory (DFT) simulations on suited models.1 Such MXenes display a high affinity towards carbon dioxide (CO2), strongly binding it, and activating it by charge transfer, gaining a bent CO2 with elongated bonds. The CCS capabilities highlighted through kinetic phase diagrams (KPD) were confirmed by experiments,2 showing a high CO2 uptake due to the MXene high surface area, specially high when MXene is made of light transition Ti or V metals. Furthermore, given the CO2 activation pristine MXenes can be used in carbon capture and use (CCU) technologies, acting as heterogeneous catalysts. A recent DFT study shows MXenes use as heterogeneous catalysts for the reverse water gas shift reaction (RWGS), where a KPD analysis reveals a swing mode RWGS operation, where CO2 is first converted into CO oxidizing the MXene surface, later regenerated by hydrogen treatment releasing water.

1 Morales-García et al. J. Mater. Chem. A 6 (2018) 3381. 2 Persson et al. Adv. Mater. 31 (2019) 1805472. 3 Morales-Salvador et al. ACS Catal. 11 (2021) 11248.

MM 51.6 Thu 11:30 A 053

Effect of Surface Terminations on the Water Intercalation into Ti3C2Tz MXene Thin Films — Aditya Sharma[1], Thierry Ouisse[1], Ulf Wiedwald[2], Andrei Chumakov[3], Fabrice Wilhelm[4], and •Hanna Pazniak[1] — [1]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France — [2]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Duisburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

MXenes are 2D materials whose surface is terminated by functional groups that drastically affect the properties of MXenes, including their affinity for water. In this study, we synthesized Ti3C2 MXenes with 1) mixed (=O, -F, and -OH) and 2) halogen (-Cl) terminations and prepared thin films by drop casting. X-ray absorption near edge structure shows different local chemical environment of Ti depending on the terminations, which is also confirmed by density functional theory. Next, we expose the MXene thin films to various humidity levels and studied the water intercalation by wide angle X-ray scattering. We observed that the interplanar spacing of mixed-terminated MXenes varied from 11.74 Å to 16.97 Å with increasing relative humidity from 0% to 100%, respectively. In the Cl-terminated MXenes, however, the interplanar spacing remains much smaller and only changes from 11.0 Å to 12.8 Å as function of relative humidity. In both cases, the process of water intercalation is reversible.

Funded by ANR-23-CE09-0031-01 project.

MM 51.7 Thu 11:45 A 053

Isotopic Analysis of Intercalated Protons in $Ti_3C_2T_x$ MXene for Electrochemical Energy Storage using in-situ FTIR Spectroscopy — •Andreas Weisser[1], Mailis Lounasvuori[1], Namrata Sharma[1], Kyle Matthews[2], Teng Zhang[2], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [2]A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

MXenes, a family of 2-dimensional transition metal carbides, are a promising candidate for use in energy storage applications due to their high capacitance. Here, we monitor the confined water and protons in $Ti_3C_2T_x$ MXene electrodes during cyclic voltammetry using operando FTIR spectroscopy. Isotopic exchange with deuterium oxide is used to allow for a better understanding of the proton dynamics inside the MXene interlayers. In-situ FTIR measurements are being performed with a dedicated electrochemical cell able to measure the different vibrational modes of the confined species. The measurements are conducted in attenuated total reflectance mode (ATR).

The focus of this presentation will be on analyzing the change of the vibrational modes of water and deuterium during electrochemical cycling versus the applied potential to the working electrode. This behaviour will be discussed with regard to the intercalation of protons and the reordering of the intercalated water or deuterium. The results will be placed in the context of MXene in the role of an electrode for pseudocapacitor applications.

MM 51.8 Thu 12:00 A 053

Electronic Structure of V2CTx MXene in aqueous solutions studied using in situ Scanning Transmission X-Ray Microscopy. — •Namrata Sharma[1], Kyle Matthews[2], Andreas Weisser[1], Mailis Lounasvuori[1], Markus Weigand[1], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie GmbH, 12489 Berlin, Germany — [2]A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering Drexel University Philadelphia, 19104 PA, USA

MXenes, a class of 2D transition metal carbides and nitrides have attracted much attention in many applications, thanks to their layered structure, hydrophilicity, and surface terminations. Recently, a new synthesis protocol has significantly improved the quality and shelf life of V2CTx MXene. This study focuses on the behaviour of V2CTx MXene in aqueous solutions studied using In-situ Scanning Transmission X-Ray Microscopy (STXM) with dedicated electrochemical flow cell at the synchrotron BESSY II. STXM provides element-specific nanomaterial electronic structure characterization in liquid at ~50nm spatial resolution. Here we characterize the electronic structure of pristine and aged V2CTx MXene in air, water, ZnSO4, and H2SO4, using X-ray Absorption Spectroscopy (XAS) at V L-edge and O K edge. The stability of individual V2CTx MXene flakes is monitored through high resolution chemical imaging over several hours in aqueous electrolyte. In this work we stress upon on the relevance of chemical imaging allowed by STXM for insights into oxidation and hydrolysis of MXene in aqueous environment at the nanoscale.

MM 52: Topical Session: In Situ and Multimodal Microscopy in Materials Physics II

Time: Thursday 10:15–12:45 Location: C 130

Topical Talk MM 52.1 Thu 10:15 C 130

Fast in situ electron tomography: nanoparticles under heat and light excitation — •Wiebke Albrecht — AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

Although standard transmission electron microscopy (TEM) makes it possible to obtain a wealth of information of static (nano)materials, an extension to measurements of dynamic structure-property relationships under realistic conditions is urgently needed. Moreover, with the emergence of nanoparticles with complex shapes, such in situ measurements need to be extended to 3D. Electron tomography (ET) allows for quantifying the 3D morphology of such nanoparticles but is inherently slow. In this talk, I will present how ET can be sped up to be compatible with in situ measurements. In addition, I will show how it can be utilized to quantify heat-induced nanoscale diffusion in single nanoparticles.

MM 52.2 Thu 10:45 C 130

In-situ study of Materials Performance and Structural Properties with high spatial resolution — Anton Davydok and •Christina Krywka — Insititute of Material Physics, Helmholtz-Zentrum Hereon, Hamburg, Germany

Over the past decade, we have seen a rapid development of materials with controlled properties for a wide range of applications from large-scale construction to nanoelectronics. This would not have been possible without a strong contribution from materials science based on experimental studies. The methods and techniques available today allow us to reconstruct the real operation and use of materials with controlled properties and characterize them in real time. In this talk, we will present the applicability and enormous potential of scanning X-ray nanodiffraction for in situ and in-operando studies. The nanofocus end-station of the P03 beamline at PETRA III (DESY, Hamburg), operated by the Helmholtz-Zentrum Hereon, offers unique conditions for in-situ and in-operando experiments in combination with X-ray nanodiffraction. The highly stable experimental setup is designed for structural analyses with submicrometer precision and allows non-destructive access to the interior and properties. The contribution of the P03 Nanofocus Endstation to materials science is demonstrated by the wide range of in-situ experiments already performed at the station, such as mechanical, thermal or electrical tests with organic and non-organic materials. Detailed technical specifications of the beamline and in-situ facilities will be presented as well as the results of the experiments.

MM 52.3 Thu 11:00 C 130

Approaching 1 ns Temporal Resolution in Time-Resolved Electron Holography by Improving Control Signals — •Simon Gaebel, Hüseyin Çelik, Tolga Wagner, Tore Niermann, and Michael Lehmann — Technische Universität Berlin, Germany

Interference Gating (iGate) is a novel and robust method for obtaining time-resolved phase information within transmission electron microscopes (TEM). Its basic idea is a time-dependent suppression of the interference pattern, realized by a deflector in the beam path to which a noise-based control signal is applied. By switching the noise on and off, an interference pattern is generated at short intervals, producing phase information from noise-free periods only.

In this presentation, a novel implementation is presented that aims to achieve increased temporal resolution approaching 1 ns due to an improved control signal. It utilizes the fact that interference patterns not only disappear in the presence of noise, but also when pi-phase shifted patterns are superimposed. The advantage of this approach is the use of square-wave-based control signals (commonly used in telecommunications), which require considerably lower amplitudes and at the same time can be hardware corrected (e.g., impedance matching).

This innovative approach makes iGate interesting for the investigation of processes at higher frequencies, as it enables the recording of phase information in the single-digit nanosecond range and opens new ways of understanding ultrafast phenomena at the nanoscale.

MM 52.4 Thu 11:15 C 130

Interference Gating - A Novel Shutter Mechanism for Time-Resolved Holography — •Tolga Wagner, Hüseyin Çelik, Simon Gaebel, Tore Niermann, and Michael Lehmann — Technische Universität Berlin, Germany

Common shutter mechanisms for realizing time-resolved imaging are usually based either on blocking the intensity of the radiation used (e.g. stroboscopic illumination) or on the fast readout time of modern detectors. For holographic investigations, which are based on the recording and reconstruction of interference patterns, a completely new type of gating mechanism is now available: interference gating (iGate).

The basic idea of iGate is a synchronized destruction of the interference pattern, realized by introducing random phase shifts to the wave, for a defined period of time during a holographic acquisition. The holographic reconstruction process acts as a temporal filter that only retains the information of the undisturbed interferogram outside this period. Since the acquisition of interference patterns is in general very susceptible to external disturbances, a targeted destruction of the interference pattern is rather easy to realize and the interference gating as a method becomes interesting in research areas, in which common shutter mechanisms are difficult to be implemented.

In transmission electron microscopy (TEM), for instance, iGate can be retrofitted with minimal technical effort in almost any existing instrument, hence transforming them into time-resolved investigation techniques at nanosecond timescales with nanometer spatial resolution.

15 min. break

Topical Talk MM 52.5 Thu 11:45 C 130

Probing the Atomic-Scale Internal Phases of Mutliferroic Domain Walls During Dynamics with In-Situ Biasining and Cryogenic STEM — •Michele Conroy — Department of Materials, London Centre for Nanotechnology, Imperial College London, Exhibition Road, London SW7 2AZ, U.K.

Dynamic multiferroic domain wall topologies overturn the classical idea that our nanoelectronics need to consist of fixed components of hardware. To harness the true potential of domain wall-based electronics, we must take a step back from the device design level, and instead re-look at the sub-atomic internal properties. With recent advances in experimental characterisation and theoretical calculation approaches, in the last 5 years reports of non-classic internal structures and functionalities within domain walls have become a common occurrence. As the region of interest is at the nanoscale and dynamic, it is essential for the physical characterisation to be at this scale spatially and time resolved.This presentation focuses on measuring the emergent phases within domain walls during dynamics via in-situ biasing 4D-STEM and EELS. Additionally to explore the low temperature magnetic phases we utilise in-situ cryogenic TEM holders.

MM 52.6 Thu 12:15 C 130

TEM-analysis of electron beam sensitive anodic aluminum oxides at cryogenic temperatures — •Lydia Daum[1], Stefan Ostendorp[1], Martin Peterlechner[1,2], and Gerhard Wilde[1] — [1]University of Münster, Münster, Germany — [2]Laboratory for Electron Microscopy, Karlsruhe, Germany

While the existence of precipitates and segregations with their related stress fields inside of aluminum alloys are essential for strengthening and achieving desired mechanical properties of these, they pose a challenge in the formation of protective anodic aluminum oxide (AAO) coatings on these. In previous studies, those precipitates are classified into three sections based on their performance during anodization. Due to methodological limitations, the experiments were carried out in enlarged intermetallic areas in binary aluminum alloys [1,2]. Here, we employ different pre-treatments to aluminum alloys, in accordance with industrial standards, to address the effect of precipitates on the formation of the electron beam sensitive AAOs. Previous scanning transmission electron microscopy (STEM) studies have shown that cryogenic temperatures can partially reduce the beam damage in materials such as AAOs [3,4]. Here, we apply multimodal electron microscopy to examine both, chemical and structural changes of the precipitates within the AAO and at the interface to the underlying alloy. This work aims for a better comprehension of AAO growth and its corresponding properties. We try to bridge the properties of aluminum alloys gained by precipitations with the optimization of the formation of AAOs, which can offer valuable insights for industrial applications.

MM 52.7 Thu 12:30 C 130

Reducing electron beam-induced defect formation by using in situ TEM gas cell — •Carina B Maliakkal[1], Paolo Dolcet[2], Lukas Braun[2], Maria Casapu[2], Di Wang[1], and Christian Kübel[1] — [1]Institute of Nanotechnology (INT) and Karlsruhe Nano Micro Facility (KNMFi), Campus North, Karlsruhe Institute of Technology (KIT), Germany. — [2]Institute of Technical and Polymer Chemistry, KIT

Ceria – a very common oxide support used in exhaust gas catalysis – was initially investigated to obtain spatially resolved quantitative information about the surface speciation. Electron energy loss spectroscopy (EELS) mapping in a Scanning Transmission Electron Microscope (STEM) was used for this purpose. We did not observe any noticeable change in the crystal structure or surface structure via simple STEM imaging. However, during our investigation to check the Ce oxidation state via EELS, we found that the extent of oxygen vacancies near the ceria surface is strongly affected by the electron beam under the TEM vacuum conditions. This is not surprising, as it is known that the electron beam can significantly alter some materials.[1] Traditional approaches to reduce electron-beam induced damage includes adjusting the high tension, electron dose and dose rate. However, since here the major damage/alteration to the ceria seems to be the induced creation of oxygen vacancies, we demonstrate that by working in oxygen atmosphere, the damage can be successfully compensated for.

Reference [1] Neelisetty et al. Microscopy and Microanalysis 2019 (25) 592.

MM 53: Data Driven Material Science: Big Data and Workflows VI

Time: Thursday 10:15–13:00 Location: C 243

MM 53.1 Thu 10:15 C 243

Scalable machine learning for predicting the electronic structure of matter — •Attila Cangi[1,2], Lenz Fiedler[1,2], Bartosz Brzoza[1,2], Karan Shah[1,2], Tim Callow[1,2], and Steve Schmerler[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Center for Advanced Systems Understanding, Görlitz, Germany

I will present our recent progress in significantly speeding up density functional theory calculations with machine learning [1], for which we have developed the Materials Learning Algorithms framework [2]. Our findings illustrate significant improvements in calculation speed for metals at their melting point. Additionally, our use of automated machine learning has yielded significant reductions in computational resources required to identify optimal neural network architectures [3]. Most importantly, I will present our latest breakthrough, which enables fast neural-network driven electronic structure calculations for systems unattainable by conventional density functional theory calculations [4].

[1] L. Fiedler, K. Shah, M. Bussmann, A. Cangi, Phys. Rev. Materials, 6, 040301 (2022). [2] J. Ellis, L. Fiedler, G. Popoola, N. Modine, J. Stephens, A. Thompson, A. Cangi, S. Rajamanickam, Phys. Rev. B, 104, 035120 (2021). [3] L. Fiedler, N. Hoffmann, P. Mohammed, G. Popoola, T. Yovell, V. Oles, J. Austin Ellis, S. Rajamanickam, A. Cangi, Mach. Learn.: Sci. Technol., 3, 045008 (2022). [4] L. Fiedler, N. Modine, S. Schmerler, D. Vogel, G. Popoola, A. Thompson, S. Rajamanickam, A. Cangi, npj. Comput. Mater., 9, 115 (2023).

MM 53.2 Thu 10:30 C 243

SE(3)-Transformers for predicting the electronic structure of hydrogen molecules — •Bartosz Brzoza and Attila Cangi — CASUS/HZDR

In this work, we demonstrate the efficacy of a neural network model implemented as the Materials Learning Algorithms (MALA) package in predicting the electronic structure of a system of hydrogen molecules under various pressure and temperature conditions across the molecular liquid-solid phase boundary, demonstrating the potential of our methods for molecular systems. Additionally, we investigate the use of SE(3)-Transformer Graph Neural Networks to improve the generalizability and extrapolation capabilities of our models. Our results indicate that the MALA framework provides a powerful and efficient tool for accelerating Kohn-Sham density functional theory calculations in molecular systems. This work paves the way for future research in developing advanced machine-learning algorithms for accelerating electronic structure calculations both accurately and efficiently.

MM 53.3 Thu 10:45 C 243

Physics-Informed Machine Learning for Addressing Challenges in Static and Time-Dependent Density Functional Theory — •Karan Shah and Attila Cangi — Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

We explore the potential of Physics-Informed Machine Learning (ML) in addressing key computational tasks in both static and time-dependent Density Functional Theory (DFT/TDDFT). The talk will focus on two projects that employ advanced ML techniques, specifically Physics-Informed Neural Networks (PINNs) and Fourier Neural Operators (FNOs), to tackle these complex tasks.

In the first part, we examine the use of FNOs in addressing the density-to-potential inversion problem in static DFT. By employing these methods as alternatives to numerical inversion schemes, we demonstrate enhancements in predictive transferability and speed. We highlight the applications to exactly solvable systems, illustrating their potential as accurate and rapid data-driven surrogate models.

In the second part, we discuss the application of PINNs to accelerate TDDFT calculations. By incorporating the fundamental physical constraints of the TD Kohn-Sham equations directly into the learning process, we demonstrate the performance and generalisability of PINN solvers on the time evolution of model systems across varying system parameters, domains and energy states.

By integrating physics and ML, these projects shed light on promising new directions for addressing challenges in DFT and TDDFT.

MM 53.4 Thu 11:00 C 243

Datadriven thermodynamic modeling with CALPHAD — •Tobias Spitaler and Lorenz Romaner — Montanuniversität Leoben, Department Werkstoffwissenschaft, Leoben, Österreich

CALPHAD models and computational thermodynamics play an essential role in materials science and in the development of novel materials. In the CALPHAD method, thermodynamic quantities and phase diagrams are calculated from a parameterized model of the Gibbs free energy, which is stored in a thermodynamic database. The reliability of the calculated quantities relies on the correctness and quality of the thermodynamic database. With new computational tools and statistical methods, the database creation can be accelerated and uncertainty can be quantified, which is propagated from the input data to the quantities of interest.

We combine heterogeneous data from experiment and simulation in CALPHAD modeling and use statistical tools to propagate the uncertainty of the model parameters to quantities of interest. We demonstrate parameter optimization and uncertainty quantification in the phase diagram of selected systems (e.g. W-Ti, Fe-C). Uncertainty quantification of phase boundaries, invariant points and other quantities of interest are demonstrated. With the statistical methods regions with high uncertainty in the composition space can be identified and the potential experiments with the highest information proposed. With the data-driven and statistical approach to CALPHAD modeling, new thermodynamic databases can be obtained in a faster and more reproducible way.

MM 53.5 Thu 11:15 C 243

Complete Basis Set Limit Extrapolation in Density Functional Theory Calculations using Statistical Learning — •Daniel Speckhard[1,2], Claudia Draxl[1,2], and Matthias Scheffler[2,3] — [1]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Berlin, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

The numerical precision of density-functional-theory (DFT) calculations depends on a variety of computational parameters, one of the most critical being the basis-set size. The ultimate precision is reached with an infinitely large basis set, i.e., in the complete basis-set (CBS) limit. Our aim is to find a machine-learning model that extrapolates

finite basis-size calculations to the CBS limit. Quantile random forests and symbolic regression, applying the SISSO approach, are used to estimate total energies, lattice parameters, and band gaps as a function of the basis-set size. The random-forest model outperforms previous approaches in the literature for both codes, while SISSO outperforms the random-forest model for the `exciting` code. Our approach also provides prediction intervals, which quantify the models' uncertainty. We evaluate our work on datasets consisting of 63 binary solids and 4000 binary semiconductors, respectively.
[1] C. Carbogno *et al.*, *npj Comput. Mater.* **8**, *69 (2022).*

15 min. break

MM 53.6 Thu 11:45 C 243

High-resolution beyond the depth of field limit in 3D phase-contrast imaging using ptychographic multi-slice electron tomography — •Andrey Romanov[1], Min Gee Cho[2], Mary Cooper Scott[2,3], and Philipp Pelz[1] — [1]Institute of Micro- and Nanostructure Research (IMN) & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich Alexander-Universität Erlangen-Nürnberg, IZNF, 91058 Erlangen, Germany — [2]University of California Berkeley, Berkeley, California 94720, United States — [3]Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

In electron microscopy, achieving atomic resolution in large volumes remains challenging, despite progress in optics and computational algorithms. Electron ptychography allows 3D information extraction from a single position- and momentum-resolved (4D-STEM) dataset, but axial resolution is limited to around 3nm. A novel approach involving tilt-series 4D-STEM data and subsequent ptychographic and tomographic reconstruction surpasses previous constraints. Here, we present the reconstruction of a phase-contrast volume three times greater than the depth of field, enabling differentiation of individual atoms in all dimensions of a Co3O4 nanocube in an 18.2 nm side length volume. This advancement opens new possibilities for material exploration in atomic-level 3D imaging.

MM 53.7 Thu 12:00 C 243

Advancing In-Situ SEM Imaging: Integrating Deep Learning Super-Resolution for Accelerated Analysis — •Tom Reclik[1], Philipp Schumacher[1], Setareh Medghalchi[1], Maximilian Wollenweber[1], Ulrich Kerzel[2], and Sandra Korte-Kerzel[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Aachen, Germany — [2]Data Science and Artificial Intelligence in Materials and Geoscience, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Aachen, Germany

Scanning Electron Microscopy (SEM) is pivotal in revealing intricate micro and nanoscale features across various research fields. However, obtaining large-area high-resolution SEM images presents challenges, including prolonged scanning durations and potential sample degradation due to extended electron beam exposure. This challenge is significantly amplified, when the time dimension in in-situ experiments is added. Here we present a new in-situ workflow, accelerating the imaging process step, by employing deep learning super-resolution algorithms coupled with the automated high resolution rescanning of points of interest. Our approach significantly speeds up the imaging process, thereby enabling the discoveries of new physics with a high statistical relevancy.

MM 53.8 Thu 12:15 C 243

Bayesian Optimization for High-Resolution Transmission Electron Microscopy — •Xiankang Tang, Yixuan Zhang, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

High-resolution transmission electron microscopy (HRTEM) allows to study the atomic structure of solid materials with a resolution of sub-Angstrom. By matching experimental and simulated images, unknown experimental parameters and crystal structures can be determined. However, this process entails strong domain expertise and can be time consuming. In this work, we implement and apply a Bayesian optimization-based approach to improve the efficiency of the image matching process. After adopting properly defined loss functions capturing both the global and local image features, it is demonstrated that our approach can not only match the experimental and simulated images in terms of absolute image contrast, but also naturally identify the unknown parameters in the experiments. This method offers a new possibility for automated HRTEM image analysis.We acknowledge Dr. Lei Jin and Prof. Rafal Dunin-Borkowski from FZ Jülich for stimulating discussions.

MM 53.9 Thu 12:30 C 243

Pydidas: A new tool for automated X-ray diffraction data analysis — •Malte Storm, Anton Davydok, Peter Staron, and Christina Krywka — Helmholtz-Zentrum Hereon, Institute of Materials Physics, Max-Planck-Strasse 1, 21502 Geesthacht

The push towards faster experiments and generally the enhanced data rates at latest generation synchrotrons require new efforts on the analysis side to keep processing speed up with experimental speed. Especially fast *in situ* or *in operando* experiments generate huge data quantities and require fast feedback (in the form of data processing) during experiments to optimize experimental results of beamtimes.

Historically, data reduction and pre-processing of X-ray diffraction datasets has been very much burden to the user groups. To help existing users and attract new user groups who do not have the technical experience to perform the required processing steps, Hereon has developed the pydidas software [1] suite for X-ray diffraction data analysis.

Pydidas is explicitly designed to allow full data analysis in a single tool, to natively process modern data container types (HDF5) and to make efficient use of parallel computing. Data browsing and display, experiment calibration, workflow setup, processing and visualization are all available from within pydidas. Emphasis has been placed on an intuitive user interface and accessibility also for non-experts. Pydidas is open source software and publicly available.

[1] http://pydidas.hereon.de

MM 53.10 Thu 12:45 C 243

Deep learning-based feature detection on 2D X-ray scattering data for high throughput data analysis — •Alexander Hinderhofer, Vladimir Starostin, Constantin Voelter, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

In situ real-time grazing-incidence X-ray diffraction (GIXD) is a key technique for thin film structural characterization during sample preparation. In-situ GIXD can produce large amounts of data, on the scale of several thousand images per hour, frequently exceeding the capabilities of traditional data processing methods. We propose an automated pipeline for the analysis of GIXD images, based on the Faster Region-based Convolutional Network architecture for object detection, modified to conform to the specifics of the scattering data. The model exhibits high accuracy in detecting diffraction features on noisy patterns with various experimental artifacts. We demonstrate our method on real-time tracking of organic-inorganic perovskite structure crystallization. By design, our approach is equally suitable for other crystalline thin-film materials.[1] Further, we discuss a high quality GIXD dataset with more than 1600 labeled features for performance evaluation of feature detection models in GIXD.

[1] V. Starostin et al. npj Comput Mater 8 (2022) 101

MM 54: Materials for Storage and Conversion of Energy V

Time: Thursday 10:15–11:30 Location: C 264

MM 54.1 Thu 10:15 C 264

Energy storage in a quantum battery — •Charles Downing — University of Exeter, Exeter, United Kingdom

We consider some simple theoretical models for quantum batteries, which are energy storage devices constructed using inherently quantum mechanical objects. We discuss the optimal ways to charge the battery, store energy in the battery and extract useful work from it. In particular, we show how quantum batteries display some nice non-Hermitian physics effects, in which so-called exceptional points govern the performance of the battery. We conclude by proposing some experimental platforms which could verify our theoretical predictions.

MM 54.2 Thu 10:30 C 264

chemically embedding cobalt nanospheres in N-doped carbon nanosheets for enhanced zinc-air batteries — •Ningxiang Wu[1], Huaping Zhao[1], Sheng Li[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Key Laboratory of Flexible Electronics (KLOFE) & Institute of Advanced Materials (IAM), Nanjing Tech University (NanjingTech), 30 South Puzhu Road, Nanjing, 211800, China

The next-generation oxygen electrochemical catalysts based on non-precious metals have been extensively studied for zinc-air batteries (ZABs). Among them, Co-N-C catalysts have attracted considerable attention due to their excellent oxygen catalytic performance. However, the synthesis of Co nanoparticles with uniform structure and distribution on conductive and stable substrates remains challenging. Herein, we have prepared cobalt nanoparticles chemically embedded in N-doped carbon nanosheets (Co@NCS) by a simple organic-inorganic hybrid molten salts method. Due to the multifunctional environment provided by the mixed salts, the Co@NCS can exhibit efficient oxygen reduction and evolution reaction (ORR/OER) performance, enabling them to be suitable in ZABs. The resulting ZABs have a considerable open-circuit voltage of 1.40 V, a good peak power density of 130.4 mW cm-2, and long cycle stability for 100 h at 10 mA cm-2.

MM 54.3 Thu 10:45 C 264

Electrodeposited manganese dioxide nanolayer on carbon cloth as a modified anode for improved zinc-based battery performance — •Dharani Madhavi Bundhooa, Jiajia Qiu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Zinc-based batteries are gaining prominence as a compelling alternative to lithium-ion batteries (LIBs), driven by their safety and environmentally friendly characteristics. However, challenges associated with Zn metal anodes, particularly the formation of Zn dendrites leading to a shortened cycle life, pose obstacles to their widespread adoption. A crucial aspect in reducing dendritic deposition of Zn involves adjusting the initial uniform nucleation, which guides subsequent uniform Zn deposition. To achieve this, a nanolayer of manganese dioxide is electrodeposited onto the surface of carbon cloth, serving as active sites for controlled nucleation and growth of metal Zn. This modified anode exhibits stable cycling performance throughout repeated Zn deposition/stripping cycles. Moreover, upon assembly into full cells enhanced electrochemical performance was obtained.

MM 54.4 Thu 11:00 C 264

Tuning Structural and Electronic Properties of MOF-5 by Ligand Substitution and Metal Node Exchange — •Joshua Edzards, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany

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 electronic properties. In this project, we perform high-throughput first-principles calculations on MOF-5. We scan all possible structures that arise by exchanging Zn with metal atoms with the same oxidation state, and by substituting the linker molecule (1,4-benzodicarboxylate) with common functional groups of varying electro-donating ability. The results of 56 different structures suggest that the atomic radius of the metal node defines the lattice constant and therefore the pore size. Earth alkaline metals and hydrogen bonds caused by the ligand substitution with COOH and OH stabilize the structure the most. Ligand functionalizations mostly affect the electronic structure by tuning the gap. In particular, linker substitution with NH_2 and OH groups lead to compounds with favorable characteristics for visible-light absorption.

MM 54.5 Thu 11:15 C 264

Advancing Energy Storage: A Study on Alkali Metal-Substituted $X_3(HITP)_2$ and $X_3(HTTP)_2$ from first principles — •Sabuhi Badalov[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology

This study delves into the potential of metal-organic frameworks (MOFs) as a sustainable alternate material for use in lithium-ion batteries. Specifically, we examine $X_3(HITP)_2$ and $X_3(HTTP)_2$ MOFs with alkali metal substitutions (Cu, Zn, Co, Ni) and functionalization by replacing oxygen with sulfur for $X_3(HTTP)_2$ MOFs and hydrogen with halogens (Cl, Br) and hydroxyl groups for all predicted structures.

Using density functional theory (DFT), we analyzed these MOFs' structural, electronic, and mechanical properties in both monolayer and bulk forms. Our study also utilized advanced machine learning techniques via force field (ML-FF) for vibrational calculations, accurately assessing the materials' stability and vibrational and thermal properties. By comparing our results with some reported experimental data, this research contributes to the theoretical understanding of MOFs. It offers practical applications for their use in portable electronics, electric vehicles, and renewable energy grids. Overall, this study highlights the potential of MOFs to revolutionize sustainable energy storage solutions.

MM 55: Liquid and Amorphous Materials II

Time: Thursday 10:15–11:45 Location: C 230

MM 55.1 Thu 10:15 C 230

Between amorphous and crystalline silicon: a revised paracrystalline model — •Louise A. M. Rosset and Volker L. Deringer — Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK

The existence of paracrystalline silicon, characterized as a crystallite embedded in an amorphous matrix, has long been a topic of debate; the argument derives from hand crafted models and a limited exploration of configurational space, restricted by slow, inaccessible quench rates.

Using a computationally efficient machine-learning potential that unlocks slow quench rates comparable to experiment, we systematically sample the space of a-Si structures by simulated melt-quenching and build a large dataset of disordered silicon configurations. This extensive database points toward the existence of 'paracrystalline' disordered structures, characterized by localized diamond-like neighborhoods that affect medium-range properties. These configurations vary widely in structure and energy, and demonstrate better agreement with experimental results than previously proposed models.

This work highlights the use of data driven methods in elucidating fundamental structural questions using systematic sampling of the configurational space.

MM 55.2 Thu 10:30 C 230

Phase Separation in Ce-Al (Ga) Metallic Glasses — •Devinder Singh[1,2] and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700 Leoben, Austria — [2]Amity School of Applied Sciences, Amity University, 226028 Lucknow, India — [3]Department of Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700, Leoben, Austria

In recent years, much attention has been given to phase separated metallic glasses (MGs) which provide a unique opportunity for designing alloys/ composites with hierarchical microstructure at different length scales. The structure and physical properties of phase separated MGs have characteristics different from those of other MGs. Many theoretical efforts have been undertaken to understand the origin of phase separation; yet the understanding of the mechanism is insufficient.

In this presentation, results of our recent studies on the role of Ga substitution in place of Al in Ce-Al (Ga) MGs will be discussed with the aim to understand the genesis of phase separation. The rationale of phase separation could not be explained in terms of enthalpy of mixing of the three possible binaries in this system. The X-ray absorption spectroscopy (XAS) spectra of Ce-based melt-spun ribbons have shown appearance of 4f0 delocalized states in Ga substituted alloys. Such a substitution has led to shortening of Ce-Ce distance in the alloys owing to chemical pressure leading to creation of two types of distinct major clusters. This work, therefore, opens up new direction of research for delineating issues pertaining to phase separation in amorphous systems.

MM 55.3 Thu 10:45 C 230

Correlations between the p content and medium-range order of bulk pd-ni-p metallic glasses — •Hongshuai Li[1], Martin Peterlechner[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Laboratory for Electron Microscopy, Karlsruhe Institute for Technology (KIT), Engesserstr. 7, 76131 Karlsruhe, Germany

So far, the understanding of a composition dependence of medium-range order (MRO) in metallic glasses is incomplete. Thus, structure-property correlations for glasses or the structural origin of often helpful *minor alloying* strategies remain unknown. In this study, we systematically investigated three as-cast ductile bulk Pd-Ni-P metallic glass samples, where the P content was deliberately varied from 17 to 21 at%. The medium-range order of these samples was characterized using variable-resolution fluctuation electron microscopy. Sampling with different parallel coherent probe sizes, so-called variable resolution FEM (VR-FEM), was performed. From the obtained normalized variance values of the experimental data the dominant MRO correlation lengths are determined. The results are discussed with respect to the compositional dependence of MRO in a given alloy system, i.e. without changes incurred by introducing additional chemical complexity.

MM 55.4 Thu 11:00 C 230

Atomic-scale model of the Invar effect in metallic glasses — •Alexander Firlus[1], Mihai Stoica[1], Pál Jóvári[2], Michalis Charilaou[3], Robin E. Schäublin[1], and Jörg F. Löffler[1] — [1]ETH Zurich, Switzerland — [2]Wigner Research Centre for Physics, Hungary — [3]University of Louisiana at Lafayette, USA

The disordered atomic arrangement of metallic glasses (MGs) provides them with a variety of unique properties such as high hardness, high strength and high elastic limit, and excellent soft-magnetic properties for Fe-based MGs. For all these properties, a microscopic explanation has already been provided, based on the disordered atomic arrangement of MGs. However, Fe-based MGs also universally exhibit the Invar effect, which reduces the coefficient of thermal expansion (CTE) in the ferromagnetic state to almost zero. Despite its universality, there has been no explanation on how the disordered atomic arrangement gives rise to the Invar effect.

We studied the atomic arrangement of quaternary MGs by in situ X-ray diffraction and absorption techniques over all length scales from the atomic to the macroscopic. Based on the experimental data we performed Reverse Monte Carlo modeling to obtain a series of 3D model structures to reveal how the magnetic interactions stabilize the atomic arrangement and lead to a reduced CTE. We find that all Fe atoms contribute to the Invar effect with their magnetic interactions, and that the structural disorder enables a local optimization of the potential energy landscape, which explains the universal occurrence of the Invar effect.

MM 55.5 Thu 11:15 C 230

Introduction of sulfur into the (Zr3Ti)(NiCu) system - characterization of a new group of Zr-based BMG containing sulfur — •Bastian Adam, Oliver Kruse, Lucas M. Ruschel, Maximillian Frey, Nico Neuber, and Ralf Busch — Lehrstuhl für metallische Werkstoffe, Saarbrücken,Deutschland

The usage of the element sulfur in Bulk Metallic Glass (BMG) synthesis was recently introduced by Kuball et al. and lead to increased research interest into these new family of BMG [1]. Here we report on the influence of sulfur on the A2B type intermetallic composition (Zr50Ti16.6Ni18.3Cu15) that was characterized by synchrotron diffraction of copper mold cast specimen to determine crystalline phases around the induced primary crystallization change. The addition enables the bulk glass forming ability (GFA) of up to 6 mm 2 at % to 3 at% sulfur. The devitrification behavior and the melting behavior was also studied by heating and melting of the samples in an in-situ synchrotron wide angle scattering experiment (WAXS) experiment utilizing a LINKAM THMS 600 furnace and a high temperature LINKAM TS1500 furnace. For the best glass former of the system the mechanical properties were investigated in terms of three-point beam bending determining the offset yield strength and breaking elongation of the alloy. [1]*A. Kuball, O. Gross, B. Bochtler, and R. Busch, *Sulfur-bearing metallic glasses: A new family of bulk glass-forming alloys,* Scr. Mater., 2018.

MM 55.6 Thu 11:30 C 230

Interplay of capillary pressure and Bangham effect during imbibition in nanopores — •Juan Sanchez[1,2], Lars Dammann[1,2], Zhuoquing Li[1,2], Laura Gallardo[1,2], Robert Meissner[1], Howard Stone[3], and Patrick Huber[1,2] — [1]Hamburg University of Technology (TUHH) — [2]Deutsches Elektronen-Synchrotron (DESY) — [3]Princeton University

We conducted water imbibition experiments in mesoporous silica glass (Vycor) using optical imaging and high-resolution dilatometry. The interplay between surface stress release (Bangham effect) and tensile Laplace pressures on the nanopore walls led to two distinct deformation regimes. Capillary filling followed the Lucas-Washburn law, exhibiting continuous expansion of the mesoporous matrix with square-root-of-the-time dynamics. Complete pore filling resulted in the sudden matrix expansion due to the disappearance of Laplace pressure. This behavior was quantitatively described by a continuum mechanical model, considering the interplay of Bangham and Laplace pressure effects in a 3D network of cylindrical pores.

We further explored the Laplace pressure contribution by conducting imbibition experiments on unsealed porous monoliths under low humidity. In this scenario, both inward (imbibition) and outward (evaporation) flows occurred simultaneously. As the in- and out-flow rates balanced, a dynamic equilibrium (artificial tree configuration) with highly curved menisci at the liquid-gas interface was observed. As a result, there is no observable disappearance of the Laplace pressure during the dilatometry experiments.

MM 56: Materials for Storage and Conversion of Energy VI (joint session MM/KFM)

Time: Thursday 11:45–13:00 Location: C 264

MM 56.1 Thu 11:45 C 264

Unraveling, with ab initio modeling, the connection between electronic structure and dynamical properties of the sodium bismuth titanate. — •Marcin Kryński — Warsaw University of Technology, Warsaw, Poland

Oxide ion solid electrolytes has have drawn significant attention as they find applications in many electrochemical devices like oxygen sensors, oxygen pumps and solid oxide fuel cells [1]. Recently, ceramic compounds based on the perovskite Na0.5Bi0.5TiO3 (NBT) attracted major attention due to its high Curie temperature (~325 °C), large remnant polarization (38 μC*cm-2) and exceptional fast oxygen-ion conduction. Interestingly, NBT shows high ionic conductivity only if the molar ration between Na and Bi atoms is above unity. Below this value, a sudden drop of conductivity is observed. In this project we employ state of the art Density Functional Theory, using Strongly Constrained and Appropriately Normed functional (SCAN) together with Dudarev approach of on-site Coulombic interaction to model oxide ion dynamics of NBT electrolyte. For the first time, we correlate dynamical properties of mobile ions with the composition-dependent presence of small polarons. Furthermore, we look at the charge transfer during dynamical processes, change of the dipole moment as well as the bond strength. All this allows us to form a coherent picture of the diffusion processes being strongly correlated to the electronic structure of the NBT and how those two aspects of this compound are modulated by the composition. This work was supported by the National Science Centre, Poland under grant number UMO-2018/30/M/ST3/00743.

MM 56.2 Thu 12:00 C 264

Exploration of Cathode-Stable Layered Solid-State Electrolytes — •Sina Ziegler, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

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

To determine a suitable halide/thiophosphate combination, we aim to identify an energetically feasible reaction pathway in the multidimensional phase diagram between the two materials. The corresponding 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. Machine-learning interatomic potentials are trained on promising material combinations to validate the approach.

MM 56.3 Thu 12:15 C 264

Understanding Anion-trapping in composite solid-state electrolytes with active ceramic fillers — •Mauricio Bonilla[1], Henry Cortes[1], Ernesto Marinero[2], Javier Carrasco[3,4], and Elena Akhmatskaya[1,4] — [1]BCAM - Basque Center for Applied Mathematics, Bilbao, Spain — [2]School of Materials Engineering, Neil Armstrong Hall of Engineering, Purdue University, West Lafayette, IN, USA — [3]Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Vitoria-Gasteiz, Spain — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Developing high-performance solid-state electrolytes (SSEs) is a key step in the development of safe and efficient solid-state batteries. Composite SSEs (cSSEs) comprising active particles dispersed in an ion-conducting polymer matrix constitute a promising strategy to obtain higher ionic conductivity (IC), and interfacial and mechanical stability than single-phase SSEs. Recent experiments showed that garnet particles enhance the IC of cSSEs and that this effect can be tuned through aliovalent doping. However, the underlying mechanism is not well understood. Here, we use an enhanced hybrid Monte Carlo technique and MD simulations to bridge this gap. By focusing on the cSSEs comprising Ga-doped $Li_7La_3Zr_2O_{12}$ particles in a polyethylene oxide (PEO) + $LiC_2F_6NO_4S_2$ (LiTFSI) matrix, we show how the dynamic electrostatic trapping of $TFSI^-$ anions leads to IC enhancement by increasing the Li^+ transference number. Moreover, we show that such enhancement can be modulated through the Ga dopant content.

MM 56.4 Thu 12:30 C 264

Can Migrating Ions Block and Deactivate the Active Sites in Solid Oxide Cells? — •Patricia König, 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

Degradation of the air electrode in electrolysis mode during the oxygen evolution reaction severely limits the commercial adoption of solid oxide cells. Up to now, the atomistic structure of this active catalyst region is essentially unknown, which prevents a detailed analysis of the actual degradation mechanisms.

In prior research, we identified a complexion at the solid/solid interface of the sintered anode [1], featuring partial amorphization and varying elemental distributions deviating from the confining bulk phases. Located around the complexion area, we propose deactivation mechanisms driven by strong cation inter-diffusion. To assess if these cation migrations impede active sites and cell functionality, we conduct a large-scale study on possible active site structural motifs. We sample structures with polarons near oxygen defects, altering ion dopant concentrations to simulate ion migration effects. By employing density-functional theory to compute EELS spectra, we link oxygen defects and their proximity to polarons to distinctive peaks in experimentally recorded EELS spectra. Ultimately, this approach aids in identifying active site structures and deactivation mechanisms, enhancing future cell design with improved efficiency and durability.

[1] H. Tuerk *et al.*, Adv. Mater. Interfaces **8**, 2100967 (2021).

MM 56.5 Thu 12:45 C 264

Anharmonic Lattice Dynamics of Solid-State Ion Conductors from Machine-Learning Molecular Dynamics — •Takeru Miyagawa, Manuel Grumet, Namita Krishnan, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

Solid-state ionic conductors (SSICs) are playing an important role in electrification of transport and energy industries. Recent studies suggested that the host lattice dynamics play a critical role in the ionic conduction mechanisms [1]. Several SSICs exhibit anharmonic lattice vibrations taking mobile ions into anharmonic regions of their potential energy surface [2, 3]. Here, we investigate the role of anharmonic host lattice vibrations and their impact on the conduction of mobile cations in SSICs by using machine-learning molecular dynamics (MLMD). Particularly, we focus on different classes of superionic conductors that all exhibit anharmonicities: AgI, a strongly disordered Ag-conductor [2]; Na_3PS_4, a Na vacancy conductor [3]; and $Li_{10}GeP_2S_{12}$, showing concerted Li migration [4]. Our results demonstrate the potential of MLMDs in understanding coupled host lattice-mobile ion dynamics and show guidelines for the design of novel SSICs with higher ionic conductivities.

[1] Zhang; Nazar Nat. Rev. Mater. 7, 389-405 (2022). [2] Brenner et al. Phys. Rev. Mater. 4, 115402 (2020). [3] Brenner et al J. Phys. Chem. Lett. 13, 25, 5938-5945 (2022). [4] Fang; Jena, Nat. Comm. 13, 2078 (2022)

MM 57: Phase Transformations III

Time: Thursday 11:45–13:00 Location: C 230

MM 57.1 Thu 11:45 C 230

Elastic precursors of the martensitic phase transition in compositionally complex NiCoMnTi alloys — David Koch[1], Benedikt Beckmann[1], Franziska Staab[1], Oleh Ivasko[2], Martin von Zimmermann[2], Karsten Durst[1], Oliver Gutfleisch[1], and •Wolfgang Donner[1] — [1]Institute of Materials Science, Technical University of Darmstadt , 64287 Darmstadt, Germany — [2]Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

Elastic precursors, such as elastic constants and phonon softening, leading to the martensitic phase transition, are of fundamental interest in understanding the mechanism behind a martensitic phase transition. This phenomenon has been extensively studied, for instance, in p-metal-containing Heusler alloys, where phonon softening along the [110] direction is commonly observed. The compositionally complex all-d-Heusler alloy NiCoMnTi exhibits a martensitic phase transition similar to p-metal Heusler alloys, even in the absence of a p-d hybridization. By studying temperature-dependent thermal diffuse x-ray scattering in single crystals, we have investigated these elastic precursors. The results shed light on the mechanism of the martensitic phase transition in all-d-Heusler alloys.

MM 57.2 Thu 12:00 C 230

Resistometric determination of GP-zone formation and growth — •Fabian Miller, Johannes Berlin, and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

Natural ageing in aluminium alloys is not yet fully understood, therefore the deeper analysis of their mechanical and electrical properties is important. These properties can be influenced by precipitate formation. Resistometry is a simple online method to monitor changes in the microstructure of a metallic alloy. In this work we focused on natural and artificial ageing of the Al-Cu system with samples containing 2 - 4 wt.% of Cu. Natural ageing depends on quenched in vacancies, so on the quenching conditions. Samples were homogenized at various temperatures and rapidly quenched to ambient temperature. Afterwards four point measurements were conducted during natural ageing. 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 other than Cu. Also the sensitivity of the setup allowed to investigate the annihilation of vacancies quenched in from different high temperatures in pure Aluminium.

MM 57.3 Thu 12:15 C 230

Bicontinuous microstructure formation through partial melting — •Zhongyang Li[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht

A bicontinuous bulk metal composite is synthesized with partial melting in this study. A single phase CuIn alloy is heated into the solid-liquid phase coexistence region at 843*C and forms an interpenetrated solid phase and liquid phase automatically. The underlying formation mechanism of this special structure is closely related to the grain boundary wetting phenomenon at high temperature. The completely and incompletely wetted grain boundaries at partial melting temperature are responsible for the connectivity of the liquid phase and the solid phase respectively. The bicontinuous structure can be preserved by quenching. Both interpenetrated solid and liquid phase can be obtained with a relatively short duration of partial melting and remain bicontinuous when exposed to prolonged heating. This research found a novel and easy method of producing bicontinuous bulk metal composite, with potential applicability to a wide range of other alloy systems.

MM 57.4 Thu 12:30 C 230

Investigation of rapid solid-state phase transformations with temperature and concentration gradients — •Stephanie Lippmann — Friedrich-Schiller-Universität Jena

The mechanism of a phase transformation depends on composition, undercooling, diffusion kinetics and the nature of the interface. Using the example of the Cu-Zn bcc phase, the high competition between different transformation mechanisms during quenching is discussed in detail based on experimental observations with temperature and concentration gradients. The investigation of the various mechanisms requires a significant level of fine-tuning. Employing one- and multidimensional, multicomponent concentration gradients and pulse heating, the conditions for diffusion controlled mechanism under kinetic effects, coupled growth, massive transformation and martensitic transformation are analysed. For pulse heating, a new device was developed and built. The high-current-low-voltage-approach allows controlled heating of low-resistance samples and a simultaneous measurement and asignment of local T-t curves and microstructures.

MM 57.5 Thu 12:45 C 230

From orbital to paramagnetic pair breaking in layered superconductor 2H-NbS2 — Davide Pizzirani[1,2], Thom Ottenbros[1,2], Maró van Rijssel[1,2], Oleksandr Zheliuk[1,2], Yulia Kreminska[3], Jasper Linnartz[1,2], Malte Rösner[2], Nigel Hussey[1,2,4], Anne de Visser[5], Jianting Ye[3], Steffen Wiedmann[1,2], and •Maarten van Delft[1,2] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, Netherlands — [2]Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands. — [3]Device Physics of Complex Materials, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands — [4]H.H. Wills Physics Laboratory, University of Bristol, Bristol, United Kingdom — [5]Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, The Netherlands

The transition metal dichalcogenide superconductors 2H-NbSe2 and 2H-NbS2 are intensively studied on account of their unique electronic properties, such as Ising superconductivity found in monolayers, with upper critical fields beyond the Pauli limit. However, interest in these materials is not limited to monolayers. Even in bulk crystals, there exist reports of multiband superconductivity and exotic states. Up to now, magnetotransport studies of these states in 2H-NbS2 are limited. Here, we report a detailed high-field mapping of the phase diagram of 2H-NbS2 by means of magnetotransport and magnetostriction. We compare bulk 2H-NbS2 and a 6 nm thick flake and find an enhanced Maki parameter in the flake, but with a reduced critical field, signifying a change of the relevant pair breaking mechanism.

MM 58: Invited Talk: Patric Huber

Time: Thursday 15:00–15:30 Location: C 130

Invited Talk MM 58.1 Thu 15:00 C 130

Liquid-Driven Nanoporous Solids — •Patrick Huber — Hamburg University of Technology, Hamburg, Germany — Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

The design of functional materials capable of adapting to changing environmental conditions can be achieved by combining soft, dynamic liquids or liquid crystals with static, nanoporous solids that act as mechanically robust scaffolds. The resulting hybrids have demonstrated unprecedented properties of stability, adaptability and response to stimuli, as desired in many applications such as robotics, microfluidics, and active metaphotonics. In nanoporous media, geometrical confinement and pore wall-fluid interaction can significantly alter the properties of the fluid, causing for example molecular structuring, large negative Laplace pressures, and altered shear viscosities. In the first part of my talk I will present opto-fluidic, X-ray and neutron scattering experiments on capillarity-driven transport, self-diffusion dynamics of liquids and aqueous electrolytes in nanoporous solids, and on the interplay between the capillarity of the liquid and the elasticity of the confining solid. The observations at the effective porous medium scale will be related to the single-nanopore behaviour, also using computer simulations. In the second part of my talk, I will show that exploiting the peculiar dynamics of liquids and liquid crystals in combination with self-organised porosity in solids offers a completely new design space for sustainable, active integrated materials with functional diversity. In particular, I will present orous hybrid materials with large electrochemo-mechanical actuation or adaptable metaphotonics.

MM 59: Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides III (joint session DS/MM/O)

Properties: Catalysis & electrochemistry; physical properties

Time: Thursday 15:00–17:30 Location: A 053

Invited Talk MM 59.1 Thu 15:00 A 053

Heterogeneous catalysis with MXenes: the role of the surface passivating groups and the structural defects — •Alexey Fedorov — Department of Mechanical and Process Engineering, ETH Zürich, CH-8092 Zürich, Switzerland

Mo2CTx, two-dimensional (2D) molybdenum carbide of the MXene family (Tx are passivating surface groups), contains only surface Mo sites and is therefore a convenient model catalyst for structure-activity studies. For instance, the catalytic activity of Mo2CTx in Fischer-Tropsch (FT) synthesis increases when a Tx coverage is minimized, the latter achieved via reductive defunctionalization of Tx groups under H2. However, high temperature H2 treatment of Mo2CTx removes also ca. one third of the carbidic lattice carbon, yielding a 2D-Mo2C1-x material that is an active methanation catalyst. The removal of Tx species is also possible in the FT conditions (i.e., in the presence of CO), and this gives 2D-Mo2C without detectable carbon vacancies and Tx groups. 2D-Mo2C material, in contrast to 2D-Mo2C1-x, converts CO to diesel range alkanes. Other examples considered include dry reforming of methane, (reverse) water gas shift as well as electrocatalytic reactions (HER, NO3RR) of Mo2CTx:M, i.e., a material with dopant sites (M = Co, Fe) replacing Mo sites in the lattice of Mo2CTx.

MM 59.2 Thu 15:30 A 053

Pt-doped Ti3C2Tx and Mo2Ti2C3Tx MXenes for catalytic hydrogenation — •Yilong Yan[1], Franck Morfin[1], Stéphane Célérier[2], and Laurent Piccolo[1] — [1]IRCELYON, CNRS & Université Lyon 1, 69626 Villeurbanne, France — [2]IC2MP, CNRS & Université de Poitiers, 86073 Poitiers, France

Transition metal carbides can act as efficient metal-like catalysts or catalyst supports, and MXenes offer renewed possibilities to anchor metal atoms and promote catalytic performances. Herein, we report on the elaboration of Pt/MXene single-atom catalysts and their performance in CO2 and alkadiene hydrogenation reactions.

Anchoring of single Pt atoms is favorable at the surface of Ti3C2Tx and Mo2Ti2C3Tx MXenes. According to in situ XAS and XPS, Pt cations partially reduce upon thermal treatment at 400 °C in H2 flow, while forming bonds with surface M atoms of the MXene. This includes the probable location of Pt atoms at M vacancies or Pt-M substitution, consistently with STEM. In addition, XAS, XRD and TPR reveal MXene restructuring together with desorption of chemical intercalants and terminal groups.

While Ti3C2Tx is inactive, Mo2Ti2C3TX exhibits significant catalytic activity for both reactions. The addition of single Pt atoms on Ti3C2Tx leads to unusually high selectivity to 2-butene from butadiene hydrogenation [Mater. Today Catal. 2023, 2, 100010]. For CO2 hydrogenation, Pt/Ti3C2Tx shows a high Pt-molar activity and almost 100% selectivity to CO; Pt/Mo2Ti2C3TX is even more active, while methane and methanol are formed as minority products.

MM 59.3 Thu 15:45 A 053

Cobalt based MXene composites for the Oxygen Evolution Reaction — •Michelle Browne — Young Investigator Group Electrocatalysis: Synthesis to Devices, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, Berlin 14109, Germany

In the Electrocatalysis: Synthesis to Devices Group at HZB, our research is focused on combining MXenes and metal oxides to create the next generation Oxygen Evolution Reaction (OER) catalysts. Metal oxides are known to be active for the OER but lack high conductivity. On the other hand, MXenes are highly conductive but oxidise readily under several conditions due to its termination sites and don't contain OER active sites. To overcome these issues, we employ several strategies in our group to combine these two materials to make one material which is OER active and high conductive. Furthermore, by blocking the MXene termination sites with a metal oxide, this may lead to less oxidation of the MXenes structure. This presentation will focus on the development of Co-based MXene materials for the OER through various fabrication methods and combining Co with other metal oxide materials (e.g. CoCu and CoRu). The OER performance of the MXene/metal oxides composites compared to their parent materials will be discussed. We will also evaluate the various strategies to one another and how the initial activity and stability of the composite materials are affected.

15 min. break

Invited Talk MM 59.4 Thu 16:15 A 053

Ultrafast Photoexcitations in 2D MXenes — •Lyubov Titova — Worcester Polytechnic Institute, Worcester, MA, USA

MXenes are 2D transition metal carbides and nitrides with electronic properties that can be tuned by their chemistry and structure. Metallic-like conductivity, flexibility, high optical damage threshold and ease of processing owing to their hydrophilicity, make MXenes candidates for a host of electronic and optical applications. We use ultrafast optical and THz spectroscopic techniques to investigate the nature and behavior of photoexcitations in MXenes of different chemistries. We show that electronic and optical properties of MXenes can be engineered by choices of the transition metals and their order as well as by controlling the intercalants in the interlayer gaps. Furthermore, we demonstrate that MXenes with high free carrier density show promise as polarizers and tunable electromagnetic interference shields in the THz range.

MM 59.5 Thu 16:45 A 053

UV-to-IR Broadband Ellipsometry Characterization of Spray-Coated MXenes — •Andreas Furchner[1], Tetiana Hryhorchuk[2], Yury Gogotsi[2], and Tristan Petit[1] —

[1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Drexel University (Nanomaterials Institute), Philadelphia, USA

The chemical composition of MXenes determines whether they exhibit metal-, semi-metal- or semiconductor-like properties, which is important knowledge regarding optoelectronic applications. We employ broadband ellipsometry to characterize the optical and structural properties of spray-coated MXene layers of different chemical composition on silicon and glass substrates. Measuring from the deep-UV (200 nm) to the mid-infrared ($25\,\mu$m) provides simultaneous access to the electronic and free-charge-carrier properties of the MXenes, as well as to their vibrational fingerprints. Furthermore, ellipsometry enables the quantification of layer thicknesses, roughnesses and film inhomogeneities. The results are corroborated by Vis microscopy and atomic-force-microscopy (AFM) measurements. The authors acknowledge support from the Federal Ministry of Education and Research in the framework of the project Catlab (03EW0015A/B) and funding from the U.S. National Science Foundation (Grant Number CHE-2318105, M-STAR CCI).

MM 59.6 Thu 17:00 A 053

2D to 3D weak localization dimensional crossover in $Ti_3C_2T_x$ MXene induced by thickness and defect engineering — •Sophia Tangui[1], Simon Hurand[1], Lola Loupias[2], Stéphane Célérier[2], Ayoub Benmoumen[1,3], Philippe Moreau[3], Marie-Laure David[1], and Vincent Mauchamp[1] — [1]Université de Poitiers, ISAE-ENSMA, CNRS, PPRIME, Poitiers France — [2]Université de Poitiers, CNRS, IC2MP, Poitiers, France — [3]Nantes Université, CNRS, IMN, Nantes, France

Due to their hydrophilic properties and very good metallic electrical behavior, MXenes are promising materials for numerous applications, including transparent conductive thin films. Therefore, there is a need to unravel the transport mechanism involved in MXene multilayers. Although weak localization (WL) has been proposed as the dominating low-temperature transport mechanism in thin films, there have been however few attempts to model quantitatively temperature and magnetic field dependent resistivity measurements.

In this talk, we will focus on the dimensionality of the low-temperature transport mechanisms in spin coated thin films elaborated with the most-studied and metallic $Ti_3C_2T_x$ MXene. The influence of the thin film thickness on one hand and of defects introduced by ion irradiation at different fluences on the other hand is studied by low temperature and magnetic field dependant resistivity measurements. The data are analyzed in the framework of both 2D and 3D models : we will demonstrate a non-trivial evolution between the two behaviors and discuss the validity of both models.

MM 59.7 Thu 17:15 A 053

Non-Covalent Functionalized Schottky Interface at Ti3C2Tx/c-Si Van der Waals Heterojunction — •Eloi Ros Costals, Sergio Giraldo, Marcel Placidi, Cristobal Voz, Joaquim Puigdollers, Edgardo Saucedo, Zacharie Jehl Li Kao, and Kunal Tiwari — Electronics Engineering Department, Polytechnic University of Catalunya (UPC), Barcelona Spain

Synergistic interaction between 2D materials and organic molecules presents an additional dimension for tuning their intrinsic properties. Herein, we aim to finely tune the work function of 2D Ti3C2Tx MXene by introducing ultrathin interlayers of organic dipoles (O.D.) with a defined dipole moment value. Interface engineering is achieved through the inclusion of poly(ethylene)amine (PEI 0.1%) and third generation poly(amido-)amine (PAMAM G3), between the Ti3C2TX and c-Si. Charge transport properties of the fabricated Schottky diodes with a structure of c-Si/O.D./Ti3C2TX were evaluated through systematic analysis of the I-V and C-V characteristics. Our investigations reveal that diodes featuring O.D. as interlayers exhibit substantially reduced reverse saturation current density (J0) and enhanced built-in potential (Vbi). We also report a significant reduction in the work function value of Ti3C2Tx from 5.8 eV to 4.2 eV for Ti3C2Tx/PEI 0.1% and 3.3 eV for Ti3C2Tx/PAMAM-G3 heterostructures. On the basis of inferences drawn from photoemission spectroscopy we ascribe this to formation of oriented interfacial dipoles at the Ti3C2Tx/O.D. interface. Our study introduces an innovative approach for precisely controlling the work function of Ti3C2Tx through the incorporation of O.D.

MM 60: Topical Session: In Situ and Multimodal Microscopy in Materials Physics III

Time: Thursday 15:45–18:00 Location: C 130

MM 60.1 Thu 15:45 C 130

Field ion microscopy contrast in Pt-Ir-Au ternary alloys — •Shalini Bhatt, Shyam Katnagallu, Felipe F Morgado, Baptiste Gault, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf Germany

Field ion microscopy (FIM) allows to resolve the position of atoms in 3D, but the atoms chemical identity can be deduced only indirectly, by local contrast variations. Utilizing our recent EXTRA-FIM approach [1], which adapts the Tersoff-Hamann approach originally developed to Scanning tunneling microscopy (STM) to tunneling-controlled ionization in FIM, we demonstrate a chemical brightness contrast in ternary alloys featuring Pt, Au, and Ir. We correlate the contrast to the electronic structure of the surface, notably the local d-band filling. Yet, the relaxation pattern observed in Au significantly influences the FIM contrast. We, therefore, explore if the contrast information from FIM can be used to correctly interpret the chemical nature and local configurations in FIM experiments. We anticipate that our approach can expand the analytical capabilities of FIM.

[1] Bhatt, S., Katnagallu, S., Neugebauer, J., & Freysoldt, C Phys. Rev. B, 107(23), 235413 (2023)

MM 60.2 Thu 16:00 C 130

Cracking Catalysts: A Synthetic Data Approach to Microscopy Image Segmentation — •Maurits Vuijk, Gianmarco Ducci, Luis Sandoval, Karsten Reuter, Thomas Lunkenbein, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

In catalysis research, the amount of microscopy data acquired when imaging dynamic processes is typically too vast for non-automated segmentation. The challenge in developing a conventional automated process is that this requires more high-quality annotated training data than available in most cases. In our approach, we thus substitute expert-annotated data with a physics-based synthetic data model.

Our electron microscopy (environmental SEM) data is collected from the process of propanol oxidation to acetone over cobalt oxide. At a certain temperature during the reaction, a phase transition occurs and cracks form on the porous surface, reducing the selectivity of the catalyst. To generate synthetic image data that approximates this transition, our algorithm composes images of the pristine room-temperature catalyst with dynamically evolving synthetic cracks satisfying two physical construction principles. First, crack growth propagates along surface paths which avoid close vicinity to nearby pores. Second, each growing path successively widens and is rendered with increasing contrast to mimic depth over several frames. We then train a neural network model with the sequential data set to obtain a segmented time series of the collected data. This novel method can be used in real-time operation to guide the microscope in capturing the initial nuclei of phase transitions within the system.

MM 60.3 Thu 16:15 C 130

Unusual field evaporation of lithium explained by first principles — •Shyam Katnagallu, Huan Zhao, Se-Ho Kim, Jörg Neugebauer, Baptiste Gault, and Shyam Katnagallu — Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany.

Lithium (Li) is a critical metal for battery operation due to its high energy density, low weight, and high mobility. To develop efficient batteries, atomic-scale characterization of complex, Li-containing materials is crucial. Atom probe tomography (APT) could provide extremely valuable insights. However, APT faces many evaporation artefacts that can render the data unusable, particularly for pure Li. We used density functional theory calculations that explicitly include high electric fields to investigate Li's field evaporation behavior from the close-packed Li(110) surface as a prototypical case. At low fields, Li preferentially adsorbs at on-top sites. We systematically study surface-diffusion of Li adatoms as a function of electric field, and discovered the existence of a

”critical” electric field below the field strength at which Li evaporates, where the on-top site becomes energetically unfavourable compared to a hollow/bridge site. This leads to a practically barrier-less diffusion of Li atoms on the surface, which explains the spotty evaporation pattern observed experimentally. To prevent this undesired effect, we explored potential approaches to minimize surface diffusion before field evaporation. One approach involves depositing a monolayer of gas such as H, N, or He, onto the Li surface. We show that such an adsorbed gas layer prevents Li atoms from diffusing on the surface.

MM 60.4 Thu 16:30 C 130

Field ion microscopy contrast for Boron in Silicon

— •Christoph Freysoldt[1], Shalini Bhatt[1], Jonathan Op de Beeck[2], Claudia Fleischmann[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf — [2]Imec, Kapeldreef 75, and KU Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium

Field ion microscopy (FIM) has been recently shown to improve atom probe tomography (APT), by imaging surface atoms prior to evaporation. This helps to elucidate dynamical surface evolution in APT, and the reconstruction artifacts that may result. In FIM, an imaging gas above the surface is ionized via electron tunneling into empty surface states. The ion flux images individual surface atoms as bright spots. The challenge in FIM is to relate contrast in gas ionization to the relevant atomic surface configurations. We study this here for the case of Boron-doped Silicon, where APT suggests an unintended clustering of the dopants. In FIM experiments with H_2 as imaging gas, a variety of bright features appears upon doping, but the nature of the surface configuration and the source of the contrast is not known. We investigate possible different surface configurations of Boron with density functional theory, as well as their appearance in FIM based on our recent EXTRA-FIM package[1]. We show that electronic structure effects cannot explain the observed bright imaging, and suggest that Boron produces exposed surface clusters during evaporation due to the high strength of Si-B bonds, that hinder homogeneous evaporation.

[1] S. Bhatt *et al.*, Phys. Rev. B **107**, 235413 (2023).

MM 60.5 Thu 16:45 C 130

A Simple and Intuitive Model for Electric Potential Distributions Around TEM-Specimens

— •Hüseyin Çelik[1], Robert Fuchs[2], Tolga Wagner[1], and Michael Lehmann[1] — [1]Institute of Optics and Atomic Physics, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

For electron holographic investigations of externally driven real semiconductor nanostructures, a good understanding of the electric potential distribution of the TEM-specimen and the resulting stray fields, especially in electron beam direction, is of great importance. Here, a simple and intuitive model for the approximation of such potential distributions inside and outside semiconductor specimens of a p-n junction, prepared by a focused ion beam (FIB), is presented. The model uses only independent convolutions of the assumed specimen core's potential distribution with a suitable kernel. This allows for the entire potential distribution of a real specimen to be inferred from only one measured projection. Consequently, a significant reduction of the required computational power as well as a drastically simplified measurement process is achieved.

Topical Talk MM 60.6 Thu 17:00 C 130

Spatially and Momentum-Resolved Vibrational Spectroscopy in the Electron Microscope

— •Benedikt Haas[1], Peter Rez[2], and Christoph Koch[1] — [1]Department of Physics & Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Department of Physics, Arizona State University, Tempe (AZ), USA

Vibrational electron energy-loss spectroscopy was already shown in the 1960s, but it took until 2014 to implement it in an actual electron microscope with sub-nm spatial resolution. This development also allowed for the exploration of larger momentum transfers.

Although optical vibrational spectroscopy techniques (in the form of tip-enhanced methods) have also reached sub-nm resolution, the electron microscope is still unique in being capable of atomically resolving bulk-like specimens, not just surfaces. Recently, we have demonstrated atomically-resolved phonon EELS of extended defects - in excellent agreement with calculations. This study has shown that grain boundaries are not only barriers to phonon transport but can also support localized phonon modes and thus potentially act as phononic waveguides.

Another promising application is momentum-resolved vibrational EELS first demonstrated in 2018. Here, we map phonon dispersion surfaces (in 2D) from momentum-resolved vibrational EELS in combination with suitable theory for quantitative comparison. The technique could be used to visualize anisotropies in phonon transport, e.g. in steady states, or to investigate mode softening.

MM 60.7 Thu 17:30 C 130

Interdiffusion-controlled phase formation at an interconnect interface during soldering

— •Sandra Gaertner, Sergiy V. Divinsky, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

Soldering is a long-standing technique to connect metal parts with a permanent bond. In this process often intermetallic compounds are formed. For the purpose of soldering, elements like Sn, Pb, Bi, Sb, Ag and Cu or their alloys are used in different compositions depending on the respective field of application. Changing environmental regulations towards lead-free solder increased the interest concerning Sn-based solder alloys. Yet, soldering of interconnects involves complex processes related to matter transport, phase stability and phase transformation kinetics. These fundamental processes might depend sensitively on local variations of the microstructure such as microstrain, dislocation accumulation, grain- and phase boundaries or voids. A rigorous analysis of the correlations between the process parameters, the resulting microstructure, the phase formation and the resulting performance necessitates detailed studies on multiple length scales. In the present work, the interdiffusion and diffusion-controlled phase formation processes in a Sn based solder alloy between a Ni based layer and a Cu substrate were investigated by quantitative scanning and transmission electron microscopy. The results are discussed with respect of the fundamental correlations between processing, defect structure and the resulting phase formation sequence.

MM 60.8 Thu 17:45 C 130

Correlative structural and thermal analysis of Zr-based bulk metallic glasses

— •Štefan Stanko[1], Jürgen Schawe[1,2], and Jörg Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Mettler-Toledo GmbH, Analytical, 8606 Nänikon, Switzerland

Bulk metallic glasses (BMGs) are metallic alloys with a disordered atomic arrangement, obtained via rapid cooling from the melt. Due to their unique properties, BMGs have recently become candidates for additive manufacturing methods such as laser powder-bed fusion (LPBF). In this work, we performed fast differential scanning calorimetry (FDSC) experiments to investigate the crystallization behavior of industrial-grade Zr-based BMGs applied in additive manufacturing. Using a modified FDSC sample holder to allow its integration into a synchrotron X-ray beam, time-temperature-transformation (TTT) diagrams were measured simultaneously with the alloy microstructure. *Ex situ* scanning electron microscopy (SEM) analysis of the samples exposed to the beam revealed that sample degradation during thermal cycling cannot be avoided even when using argon atmosphere. Therefore, TTT diagrams measurements were also performed in a device integrating the FDSC within an SEM, to investigate the degradation *in situ*. The results were correlated with the oxygen content of the alloys to optimize the additive manufacturing process.

MM 61: Liquid and Amorphous Materials III

Time: Thursday 15:30–16:45 Location: C 243

MM 61.1 Thu 15:30 C 243

Spectroscopic imaging pump-probe ellipsometry on fused silica after femtosecond laser irradiation — •Theo Pflug, Markus Olbrich, and Alexander Horn — Laserinstitut Hochschule Mittweida, 09648 Mittweida, Germany

Focused ultrashort-pulsed laser radiation enables the processing of transparent dielectrics such as glass even if the photon energy is lower than the energy band gap of the material. The underlying nonlinear physical processes, namely multiphoton-, tunnel-, and avalanche-ionization, have already been investigated in numerous experimental and theoretical studies and depend strongly on the transient optical properties of the material during irradiation. In this paper, we present a pump-probe setup combined with an imaging ellipsometer that allows to measure the transient complex refractive index of the excited material with a temporal, spectroscopic, and spatial resolution. The comparison of the measured transient optical properties of fused silica with various theoretical models for describing the dielectric function from the literature allows the validation of these models, and therefore a better insight into nonlinear excitation processes.

MM 61.2 Thu 15:45 C 243

Evaluation of optical anisotropy on the surface of stressed glass using a reflective polarimetric setup — •Felix Müller, Hainer Wackerbarth, and Georgios Ctistis — Institut für Nanophotonik Göttingen, Hans-Adolf-Krebs-Weg 1, 37077 Göttingen

The rising requirements on glass in its wide range of usage embrace stability and functionality. An important factor to achieve these is the precise adjustment of desired or undesired residual stress corresponding to the application. In order to determine surface stress with a non-contact, non-destructive and automatable method we have come up with a polarimetric approach. In contrast to the well-established transmission polarimetry, the challenge to be surface sensitive demands a much higher resolution of polarisation states and a more complicated measurement data analysis due to the oblique incidence. We have managed to distinguish surface stress differences in the range of 1 MPa by applying external stress for different orientations of two of the principle axes in the surface plane. Furthermore we have reached a spatial resolution of the laser spot size of 1 mm and are able to scan qualitative stress maps on certain areas of the sample's surface. The polarimetric surface stress measurement considers the relation between the incoming and outgoing polarisation state. A comparison enables to refer the measured state to the material's reflection properties, as described by a reflection matrix in the Müller-Stokes-formalism. Therefore, quantifying surface stress from those measurements underlies, additionally to a sufficient set of measured parameters, the relation between the Fresnel reflection matrix and the type and reason of the sample's anisotropy.

MM 61.3 Thu 16:00 C 243

X-ray photon correlation spectroscopy on metallic glass formers under non-isothermal temperature scan conditions — •Maximilian Frey[1], Ralf Busch[1], and Eloi Pineda[2] — [1]Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany — [2]Department of Physics, Institute of Energy Technologies, Universitat Politècnica de Catalunya - BarcelonaTech, 08019 Barcelona, Spain

Using high flux synchrotron radiation (ESRF, ID10), we study a Pt-based metallic glass former via X-ray photon correlation spectroscopy (XPCS) upon temperature scanning through the glass, glass transition and supercooled liquid (SCL). In the equilibrium SCL, the obtained intensity autocorrelation functions, g2, are well-described by a conventional Kohlrausch-William-Watts (KWW) model. Yet, in the glass and especially the glass transition region, this approach fails. Instead, we demonstrate that a multiplication of two KWW functions allows to describe the complex decay shape. Within the glass transition region, the fit parameters of the two separate KWW fits decouple massively. While one KWW component models the compressed shape of glass-typical non-equilibrium dynamics, the other fit maintains stretched liquid-like characteristics. We demonstrate that the compressed decay can be likely addressed to ballistic-like atomic motions while the stretched component apparently reflects (sub-)diffusive atomic motions, which are both superimposed in the non-equilibrium.

MM 61.4 Thu 16:15 C 243

In-situ measurement of thermodiffusion in liquid alloys — •Elke Sondermann, Asbjørn Krüger, and Andreas Meyer — Institute of Material Physics in Space, German Aerospace Center (DLR), 51147 Cologne, Germany

Thermodiffusion, also called Soret effect, describes the formation of a concentration gradient induced by a temperature gradient. This cross-coupling effect of heat and mass transfer influences the homogeneity of doped semiconductors and grown crystals as well as the microstructure formation in alloys. The calculation of thermodiffusion by molecular dynamic simulation can be very sensitive to the specific potential. To validate models for thermodiffusion in liquid alloys, reliable measurements are needed.

Using x-ray radiography in combination with a high temperature furnace, thermodiffusion in liquid Al-Ag has been measured. This technique enables in-situ observation which excludes disturbances by solidification and reveals possible error sources as e.g. free surfaces. Thanks to the time-resolved information from x-ray radiography, the interdiffusion coefficient could simultaneously be measured and is in good agreement with previous interdiffusion measurements in this concentration range. The measured Soret coefficient is compared with the values predicted by the current theoretical models, which are found to be off by at least a factor of two.

MM 61.5 Thu 16:30 C 243

Fe and Zr diffusion in columnar Cu-Zr nano-glasses — •Christian Aaron Rigoni[1], Hendrik Voigt[1], Evgeniy Boltynjuk[2], Anoosheh Akbari[1], Bonnie Tyler[3], Sergiy Divinski[1], Harald Rösner[1], Horst Hahn[2,4], and Gerhard Wilde[1] — [1]University of Münster, Institute of Materials Physics, Münster, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [3]University of Münster, Physikalisches Institut and Center for Soft Nanoscience, Münster, Germany — [4]University of Oklahoma, CBME and AME, Norman, OK73019, US

The concept of nano-glasses is to combine the beneficial characteristics known from defects in a crystalline material with an amorphous structure of a glassy alloy, with a focus on the presence of glass-glass interfaces. The presented study investigates anomalous diffusion along such interfaces in magnetron-sputtered Cu60Zr40 columnar nanoglasses. A combination of the radiotracer technique and time-of-flight secondary ion mass spectroscopy is used to measure the solute diffusion of Fe and self-diffusion of Zr atoms. The obtained results are directly compared to a homogenous glass with a similar composition, revealing enhanced diffusivities which are interpreted in terms of an excess free volume located at the glass-glass interfaces. The diffusion studies are directly supported by the structural observations made by TEM, documenting the existence of two different amorphous phases and correspondingly glass-glass interfaces in the columnar Cu-Zr nanoglass.

MM 62: Developement of Calculation Methods III

Time: Thursday 15:45–18:00 Location: C 264

MM 62.1 Thu 15:45 C 264

Phase transitions in radial distribution biased Molecular Dynamics simulations — •Lars Dammann[1,2], Patrick Huber[1,2], and Robert H. Meissner[1,3] — [1]Hamburg University of Technology, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Molecular Dynamics (MD) simulations are crucial for the study of phenomena at the atomic level. However, simulating the transition from liquid to solid states remains a challenge due to the energy barrier between phases, that makes the observation of spontaneous phase transitions in unbiased simulations computationally infeasible. Radial distribution functions (RDFs) provide valuable insights into atomic structures but are not unambiguous and therefore hard to interpret. I will present an algorithm that biases molecular dynamics simulations to reproduce a target RDF while minimizing the amount of information with which the original force field is biased. This is achieved through the application of the principle of maximum relative entropy. Following this principle, it is possible to use the structural information about the system contained in the RDF while conserving as much information as possible about the atomic interactions contained in the original force field. I will demonstrate that this strategy can be used to promote liquid-solid phase transitions in MD simulations. In the future, this method could potentially aid in the investigation of complex phase transitions, the analysis of metastable states and for the interpretation of structural information from experimental data.

MM 62.2 Thu 16:00 C 264

Finite temperature electronic structure calculations for heavy element tetrahedral semiconductors using a dynamic tight-binding model — •Shaoming Zhang, Martin Schwade, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

Performing first-principles calculations of electronic properties at finite temperatures typically involves a substantial computational effort. Recent advancements in machine learning force-field molecular dynamics have expanded our ability to simulate large systems over longer timescales. But accurately computing the electronic structure in large, thermally disordered materials, particularly with non-negligible spin-orbit coupling effects when heavy elements are involved, remains difficult. To tackle these computational challenges, our approach adapts the tight-binding formalism for enhanced efficiency. Central to our method[1] is the use of hybrid-orbital basis functions, along with the incorporation of spin-orbit coupling. This yields a dynamic tight-binding model defined by a small set of parameters, optimized through density functional theory calculations. We show that our model is able to describe the temperature-dependent electronic properties of tetrahedral semiconductors with heavy elements, demonstrating alignment with first-principles results.

[1] M. Schwade, M. J. Schilcher, C. Reverón Baecker, M. Grumet, D. A. Egger, arXiv:2308.08897 [cond-mat.mtrl-sci] (2023)

MM 62.3 Thu 16:15 C 264

Machine Learning Potentials for Multi-State Systems: Predicting Photoluminescence Spectra from Molecular Dynamics — Christopher Linderälv[1,2], •Nicklas Österbacka[2], Julia Wiktor[2], and Paul Erhart[2] — [1]University of Oslo — [2]Chalmers University of Technology

Divacancy defects in 4H-SiC show potential as single-photon emitters, which are important devices in quantum information technology. The photoluminescence spectra of these defects are crucial for this application, and accurate prediction of such spectra can aid in both understanding of the underlying defect physics and in device optimization.

We introduce a method for predicting photoluminescence spectra from the energy difference between the ground and excited state of defects sampled from molecular dynamics (MD) simulations, for which we employ machine learning potentials (MLPs) to extend the accessible length and time scales. Standard MLP construction approaches lead to exponential divergence in absorption and emission energies with increasing system size, however. To circumvent this, we introduce a method for the construction of MLPs capable of simultaneously describing both states.

We construct such a potential for a 4H-SiC divacancy defect and show that our MD-based approach yields emission spectra in good agreement with the generating function approach, which is the gold standard for such predictions from atomic structure. We also highlight the advantages of our MD-based method, emphasising synergies with MLPs.

MM 62.4 Thu 16:30 C 264

Dynasor 2.0: From simulation to experiment through correlation functions — •Esmée Berger, Erik Fransson, Fredrik Eriksson, Eric Lindgren, and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Using correlation functions, the full dynamics of a system can be accessed from atomistic simulations. This is particularly relevant for systems where perturbative approaches are not applicable, including liquids, metastable crystal structures, and anharmonic materials. The dynasor package is a flexible and efficient tool for calculating correlation functions, such as static and dynamic structure factors, both partial and total, as well as current correlation functions. Crucially, correlation functions provide a bridge to experiment, as weighing them with cross sections (or form factors) of, e.g., neutrons, X-rays or electrons, allows for the direct prediction of experimental spectra. Here, we demonstrate the new functionalities of dynasor 2.0, now featuring a Python interface, direct support for weighing, and the ability to handle trajectories from more molecular dynamics packages than before. The utility of dynasor is demonstrated through a wide range of examples, including static and dynamic structure factors, different experimental spectrum predictions, and phonon dispersions, for systems ranging from liquid Al to perovskite BZO.

MM 62.5 Thu 16:45 C 264

Machine-learned interatomic potential for microstructure formation in Ni-rich NiAl systems — •Adam Fisher[1], Julie B. Staunton[1], Huan Wu[2], and Peter Brommer[1] — [1]University of Warwick, Coventry, UK — [2]TWI 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 explored using kinetic Monte Carlo (kMC) studies. This requires reliable values for the barrier energies separating distinct atomic configurations. We have previously described a method to find and validate barriers in this system and found that classical potentials such as embedded-atom method (EAM) fail to reproduce the correct ordering of barriers. Modern machine-learned interatomic potentials (MLIPs) have been shown to have an accuracy near that of density functional theory (DFT) at a fraction of the cost. In this work, we fit an atomic cluster expansion (ACE) MLIP for nickel-rich NiAl systems using ACE hyper-active learning (ACEHAL), training on a series of structures, from cubic unit cells of Ni and Ni_3Al to large ($>$ 100w atoms) NiAl solid solution cells. This is complemented by HAL runs on saddle point configurations, which improve the description of energy barriers. The MLIP barriers are then validated and compared to several traditional interatomic potentials.

MM 62.6 Thu 17:00 C 264

Cross-Platform Hyperparameter Optimizer for Machine-Learning Potential Fitting — •Daniel F. Thomas du Toit, Yuxing Zhou, and Volker L. Deringer — Department of Chemistry, University of Oxford, Oxford, UK

The use of machine learning interatomic potentials (MLIPs) to study materials has become increasingly popular in recent years. As the field has matured, multiple frameworks for MLIP fitting have been proposed. Here we present a Python package to optimize hyperparameters for MLIPs.

Our package, XPOT (“Cross-platform optimizer for machine learning interatomic potentials”), uses bespoke interfaces to MLIP fitting programs. XPOT enables users to use automated optimization to fit robust, accurate, and fast MLIPs. Using XPOT, we optimized hyperparameters for SNAP and ACE potentials based on existing training databases for Gaussian approximation potential (GAP) models, and demonstrated cost improvements while retaining high accuracy. We showcase the usefulness of the approach by creating optimized MLIPs across a diverse range of complex materials systems.

MM 62.7 Thu 17:15 C 264

Warm Dense Hydrogen as a Benchmark for Machine-Learning Potentials — Bastian Jäckl[1], Thomas Bischoff[1], and •Matthias Rupp[1,2] — [1]University of Konstanz, Germany — [2]Luxembourg Institute of Science and Technology, Luxembourg

Machine-learning potentials (MLPs) are fast data-driven surrogate models of potential energy surfaces that can accelerate ab-initio dynamics simulations by several orders of magnitude. The performance of MLPs is commonly measured as the prediction error in energies and forces on data not used for training. While low prediction errors on a test set are necessary, they are not sufficient for good performance in dynamics simulations. The latter requires physically motivated performance measures obtained from running accelerated simulations. The adoption of such measures, however, has been limited by the effort and domain knowledge required to calculate and interpret them. To overcome this limitation, we present data and scripts to automatically quantify the performance of MLPs in dynamics simulations of hydrogen under pressure. For this challenging benchmark system, we provide geometries, energies, forces, and stresses, calculated at the density functional level of theory for different temperatures and mass densities. We also provide scripts to automatically calculate, quantitatively compare, and visualize pressures, diffusion coefficients, stable molecular fractions, and radial distribution functions. Employing our benchmark, we show that several state-of-the-art MLPs fail to reproduce a crucial liquid-liquid phase transition, despite low test set errors in energies and forces.

MM 62.8 Thu 17:30 C 264

Ab initio Raman spectroscopy including temperature: Theory and application for GaN and BaZrS3 — •Florian Knoop[1], Nimrod Benshalom[2], Matan Menahem[2], Omer Yaffe[2], and Olle Hellman[2] — [1]Linköping University, Sweden — [2]Weizmann Institute of Science, Israel

Ab initio simulations of Raman spectroscopy are often performed within the harmonic approximation, which is insufficient for describing realistic spectral properties of materials. Here we present a numerically efficient scheme that couples ab initio simulations, equivariant neural network potentials, and self-consistent phonon theory in the temperature-dependent effective potentials (TDEP) framework to perform precise simulations of Raman response at finite temperature. The method is presented for wurtzite GaN in comparison to latest experimental results, with a focus on rigorous treatment of direction and polarization-orientation (PO) dependence in optically anisotropic solids with LO/TO splitting, which is often neglected in computational approaches. Subsequently we discuss BaZrS3, a highly polarizable yet lead-free chalcogenide Perovskite with strong optical response to showcase the approach for complex materials. Overall, we find excellent agreement with experiment for both materials and show how the polarization information can be used e.g. to discern crystallographic orientations. We conclude by discussing limits and systematic errors in the approach with implications for other materials simulations, as well as possible strategies to overcome some of them by tighter integration of experiment and theory.

MM 62.9 Thu 17:45 C 264

An efficient method for estimating the dynamics of full polarizability tensor in *ab initio* molecular dynamics simulations — •Pouya Partovi-Azar — Martin Luther University of Halle-Wittenberg, Halle (Saale), Germany

An efficient method is presented to approximate the dynamics of individual polarizability tensor elements, for example during *ab initio* molecular dynamics simulations. The method is based on the calculation of quadrupole moment matrix of the position operator in maximally-localized Wannier functions representation. The presented method has a wide range of applications, particularly in vibrational spectroscopy simulations, such as (resonance) Raman, Raman optical activity, sum-frequency generation, etc. It is demonstrated that this method can lead to several hundred times speedup with respect to reference linear response calculations. The predictive power of the introduced method is tested in case of various molecules as well as depolarized Raman spectra of gaseous and liquid methanol, in all of which remarkable agreements with the reference spectra are observed.

MM 63: Functional Materials: Performance, Reliability and Degradation

Time: Thursday 15:30–16:45 Location: C 230

MM 63.1 Thu 15:30 C 230

Combining DFTB and Structure Mapping for the Prediction of Transition Paths in the Deactivation of ZnO@Cu Catalysts — •Artem Samtsevych, Chiara Panosetti, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Solid-solid transformations are common in the aging of functional materials like catalysts. Understanding these transformations at the atomistic level is thus crucial for a resilient design. In practice, this requires identifying minimum energy pathways between basins on a complex free energy surface. While chain-of-state methods help obtain corresponding pathways, they are generally challenged by the exponential growth of the number of possible transition pathways with system size and the computational cost of the underlying first-principles, typically density-functional theory (DFT), energy evaluations.

Here we address both challenges by employing geometry- and topology-based mapping techniques for the efficient generation of suitable initial transition pathways and a machine learning-based optimization of density-functional tight binding (DFTB). The former techniques map the atomic structures and unit cells or the graphs of interatomic bonds of the connected basins. The latter optimization of the DFTB repulsive potential [1] establishes this technique as a computationally efficient surrogate for the DFT energetics. We illustrate the combined general workflow by studying the aging process in ZnO@Cu catalysts, which involves the transformation of the ZnO overlayer from a graphitic-like to wurtzitic structure.

[1] C. Panosetti *et al.*, J. Chem. Theory Comput. **16**, 21818 (2020).

MM 63.2 Thu 15:45 C 230

Structural and chemical behavior of cBN at high pressure and temperature — •Lars Olschewski[1], Gabriel Brune[1], Tountzer Dereli[2], Monika Kipp[2], Dirk Biermann[2], and Jörg Debus[1] — [1]Department of Physics, TU Dortmund — [2]Institute of Machining Technology, TU Dortmund

Solids need to withstand high temperatures and heavy forces while they are used in extreme thermo-mechanical environments, like high-speed precision-grinding applications. Cubic boron nitride (cBN) is commonly exploited as abrasive material, because it is structurally stable and resistant to oxidation typically until temperatures of 1300°C.

For applying strong normal and tangential forces (tens of N) and high temperatures, the mechanically most stable (sp^3-hybridized) cBN may change into its hexagonal form or its crystal structure may transform into an amorphous mixture of stressed and anisotropic sp^2- and sp^3-hybridized bonds. In that context, studying the anisotropies in the tensile, compressive and shear strain as well as surficial chemical reaction products is highly interesting.

This structural and chemical behavior is investigated by confocal Raman scattering and tip-enhanced Raman spectroscopy. They allow for sensitively characterizing topographic features at the nanoscale combined with data on, *e.g.*, the chemical composition.

MM 63.3 Thu 16:00 C 230

Optimizing In_3SbTe_2 crystallization towards phase change memory application — •Yiming Zhou and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074, Aachen, Germany

Traditional phase change materials like $Ge_2Sb_2Te_5$ are characterized by their low crystallization temperatures, resulting in insufficient data retention. In contrast, In_3SbTe_2, an indium-based chalcogenide, exhibits remarkable characteristics including notably high crystallization temperatures and resistance contrasts. However, its multi-stage crystallization process has raised challenges to switching reliability and device endurance. To address this problem, an investigation into the crystallization behavior of In_3SbTe_2 through controlled annealing processes has been conducted.

The large density changes during the crystallization process and the as-deposited crystallite contribute to the adhesion problem. This gives rise to the strain relaxation-induced crystallization behavior. With the Te adhesion layer, the operational stability range for In_3SbTe_2 crystallization can be significantly expanded. Moreover, manipulating the thickness of the Te adhesive layer can tune the preferred orientation for In_3SbTe_2 crystallization.

This refined crystallization study has culminated in the fabrication of confined and nano-bridge phase change memory devices. Notably, a marked enhancement in yield has been observed for both device architectures, representing substantial progress toward practical implementation.

MM 63.4 Thu 16:15 C 230

Thermomechanical properties of diamond abrasive grains — •Gabriel Brune[1], Tountzer Dereli[2], Lars Olschewski[1], Monika Kipp[2], Dirk Biermann[2], and Jörg Debus[1] — [1]Department of Physics, TU Dortmund — [2]Institute of Machining Technology, TU Dortmund

Abrasive grains are subjected to high thermomechanical stress during high-speed precision grinding. While cubic boron nitride is often used for its high hardness and thermal resistance, diamond - with its superior hardness - provides better grinding results. However, when machining steel at temperatures of about 600°C, graphitization of the diamond surface is a major issue lowering the structural and chemical stability.

These structural and chemical changes including the influence of O_2 and interfaces between sp^2 and sp^3 hybridized areas within the carbon network are in the focus of our studies. Accordingly, a series of diamond abrasive grains exposed to differently high thermomechanical loads was analyzed. Spatially resolved Raman spectroscopy of the diamond surface reveals the structural properties of the grains. Based on shifts of the diamond Raman peak at 1332 cm^{-1}, tensile and compressive strain up to 200 MPa is determined. In particular, the observation of the D peak (around 1350 cm^{-1}) and G peak (around 1550 cm^{-1}) indicates the local formation of amorphous carbon clusters. From the peak shapes it is possible to estimate local maximum surface temperatures (= 660°C) [APL Mater. 11, 031106 (2023)] that occured during the grinding process.

MM 63.5 Thu 16:30 C 230

Influence of flash lamp annealing on the martensitic microstructure of epitaxial Ni-Mn-Ga films — Yuru Ge[1,2], Satyakam Kar[3,2,1], Fabian Ganss[1], Thomas Schumann[1], René Hübner[1], Lars Rebole[1], and •Sebastian Fähler[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden — [2]TU Dresden, Faculty of Mechanical Science and Engineering, 01062 Dresden — [3]Leibniz IFW Dresden, Institute for Metallic Materials, 01069 Dresden

The application of shape memory materials are based on a reversible martensitic transformation, which changes structure and microstructure. All applications like high stroke actuation, sensing, ferroic cooling, and energy harvesting, benefit from a high cycle frequency, as this allows for high power density. For this, thin films are of particular interest as their high surface-to-volume ratio enables fast heating and cooling. However, up to now the influence of fast heating and cooling on the martensitic microstructure is unknown. Here we examine the influence of flash lamp annealing on epitaxial Ni-Mn-Ga films. Single-crystalline films are suitable as a model system since they allow for an undisturbed, well-ordered hierarchical martensitic microstructure after slow cooling. We examine all levels of this twin-within-twins microstructure by a combination of XRD, SEM and TEM before and after flash lamp annealing with a duration of 3 ms at different energy densities. We observe substantial changes at all levels of twinning, which we attribute to the finite time available to form a hierarchical microstructure and the thermal stress between film and substrate.

MM 64: Liquid and Amorphous Materials IV

Time: Thursday 16:45–18:00 Location: C 243

MM 64.1 Thu 16:45 C 243

Machine learning quantum Monte Carlo: application to water clusters — •Matteo Peria, Michele Casula, and Antonino Marco Saitta — IMPMC, Sorbonne Université, CNRS, MNHN, UMR 7590, 4 Place Jussieu, 75252 Paris, France

A complete understanding of the hydrogen bond and proton transfer mechanism in water is still lacking, since it requires an accurate potential energy surface (PES) and very expensive quantum mechanical simulations of the nuclear part. Reproducing this high-dimensional surface with current high-level computational chemistry methods is infeasible for the largest clusters. We test gradient-based kernel ridge regression methods and neural networks to reproduce the PES starting from a dataset of energies and forces of the protonated water clusters obtained via simulations combining classical molecular dynamics (MD) for the nuclei and quantum Monte Carlo (QMC) for the electrons. The QMC+MD approach yields very accurate results for the classical dynamics, which are however affected by the intrinsic noise inherent in the stochastic sampling of both nuclear and electronic phase space. We prove that QMC multivariate noise is not detrimental to the learning of energies and forces and that the derived machine learning force field can be used to run long and reliable quantum molecular dynamics simulations.

MM 64.2 Thu 17:00 C 243

Device-scale atomistic modelling of phase-change memory materials using a machine-learned interatomic potential — •Yuxing Zhou[1,2], Wei Zhang[2], En Ma[2], and Volker L. Deringer[1] — [1]Department of Chemistry, University of Oxford, UK — [2]Center for Alloy Innovation and Design, Xi'an Jiaotong University, China

Phase-change materials (PCM) are leading candidates for next-generation memory and neuromorphic computing chips. The Ge–Sb–Te alloys on the GeTe-Sb2Te3 tie-line (referred to as “GST”) have been most widely studied and used in commercial memory products. Quantum-accurate computer simulations have played a central role in understanding complex GST alloys. However, the large computational cost has precluded simulations on the length scales of real devices. In this presentation, we describe a single, compositionally flexible machine-learning interatomic potential with a quantum-mechanical level of accuracyy. We show that our model can describe the flagship GST alloys under various practical device conditions, e.g., non-isothermal heating, and taking chemical disorder into account. The superior computing efficiency of the new approach enables the simulation of multiple thermal cycles. We also show a device-scale capability demonstration in a real device model of more than 500,000 atoms. These describe technologically relevant processes in realistic memory products. Our work demonstrates how atomistic ML-driven simulations can help study the structural and chemical properties as well as programming mechanisms of GST devices.

MM 64.3 Thu 17:15 C 243

Towards in-depth atomistic understanding of polymer-derived silicon oxycarbides using machine-learning potentials — Niklas Leimeroth, •Jochen Rohrer, and Karsten Albe — Institute of Materials Science, Technical University Darmstadt, Otto-Berndt-Strasse 3, 64287, Darmstadt, Germany

Polymer-derived amorphous silicon oxycarbides (SiOC) show promising properties for advanced applications in a variety of fields such as high-temperature coatings, biomedicine and batteries. This outstanding versatility is due to their highly tunable composition and microstructure. Simultaneously, this tunability poses a challenge for a thorough knowledge and understanding of structure-property relations in this system. In this work, we present a machine-learning potential (MLP) for SiOCs based on the atomic cluster expansion (ACE) and trained to a diverse set of actively-learned density functional theory (DFT) data. We demonstrate the capability of the MLP to model glass-phase and microstructure formation from commonly used polymer-precursor fragments, contrast these microstructures with experimental findings and show how atomistic simulations can be used to understand complex structure-property relations on the example of Young's Moduli in relation to phase volumes and different types of bonding in the system.

MM 64.4 Thu 17:30 C 243

Modelling amorphous forms of complex hybrid-inorganic

frameworks — •Thomas C. Nicholas, Daniel F. Thomas du Toit, Andrew L. Goodwin, and Volker L. Deringer — Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK

With the continued development of efficient fitting and evaluation frameworks for machine learning potentials (MLPs), modelling complex, multi-component materials is now possible. However, for systems built up of metal nodes connected by organic linkers, such as metal-organic frameworks (MOFs), the time-scales and length-scales required to model and label representative amorphous training configurations using traditional database generation strategies (for example, ab initio molecular dynamics and iterative training) remains a challenge.

We demonstrate a two-stage approach to tackle this, focusing on modelling the amorphous form of a MOF built up from Zn nodes and imidazolate linkers ($Zn[C_3N_2H_3]_2$). Firstly, by exploiting the structural analogy between silica networks and this MOF, we construct a topologically and geometrically diverse database of configurations through a back-mapping scheme whereby we decorate AB_2 networks with Zn nodes and imidazolate linkers. Secondly, we introduce an iterative training protocol whereby training configurations are generated using a Monte Carlo simulation refinement that seeks to minimise the difference between the computed and experimental data.

In this way, we demonstrate how our MLP better describes possible amorphous configurations.

MM 64.5 Thu 17:45 C 243

Thermodynamic Assessment and CALPHAD Simulation of the Ni-Pd-S Glass Forming Ternary System — •Maryam Rahimi Chegeni[1], Wenhao Ma[2], Sascha Riegler[1], Amirhossein Ghavimi[1], Magnus Rohde[2], Hans Jürgen Seifert[2], Isabella Gallino[3], and Ralf Busch[1] — [1]Saarland University, Chair of Metallic Materials, Germany — [2]Karlsruhe Institute of Technology, Institute for Applied Materials-Applied Materials Physics, Germany — [3]Department of Materials Science and Engineering, Metallic Materials, TU-Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, Germany

This work conducts an experimental and computational investigation into the thermo-physical properties of the novel ternary BMG-forming Ni-Pd-S system. The simplicity of the ternary Ni-Pd-S BMG-forming system facilitates the application of the CALPHAD approach for the modeling of the underlying thermodynamics affecting the glass formation.

Experimental quantitative specific heat capacity and crystallization studies of glass-forming compositions are performed to assess thermodynamic parameters and generate input data for the calculations and modeling of the undercooled liquid. Using the two-state approach , the modeling of the undercooled liquid and glass for the pure elements and the corresponding ternary system is done.

Subsequently, the evaluation of the glass forming ability of the system is performed using the parallel tangent method for Gm of the crystalline and the liquid phases and the results are used for modeling the isothermal TTT diagrams.

MM 65: Additive Manufacturing: Microstructure Development

Time: Thursday 16:45–18:00 Location: C 230

MM 65.1 Thu 16:45 C 230

Atomistic Simulations of Laser-based Powder Bed Fusion — Fabio Oelschläger[1], Azad Gorgis[1], Jonas Schmid[1], Kevin Vietz[1], Dominic Klein[1], Sarah Müller[2], and •Johannes Roth[1] — [1]FMQ, Universität Stuttgart, Germany — [2]GSaME, Universität Stuttgart, Germany

Applications of additive technologies continue to demand an improvement in quality and reproducibility. Using atomistic molecular dynamics simulations we are able to better understand the root causes for defects and may also be able to derivate actions for defect avoidance. The biggest challenge to the simulations are the scales: although we use multi-million atom systems and run “long” simulations we have to scale parameters like particle size, laser power, power density, scanning speed, laser focus diameter and gravity.

Using parameter studies for scanning speed and laser power while also including the influence of protective argon gas, different inclusion defects in pure aluminum particles are shown. The simulation of powder beds formed by spheres of different sizes show holes which vanish if filled with vacuum but persist if the simulation box is filled with protective gas allowing insight into the defect formation. Recrystallization in a box filled with a bimodal distribution of aluminum particles has been observed. Additionally, different configurations of binary materials made of aluminum and titanium have been simulated: the study compares spheres formed by a core of aluminum and an outer shell of titanium or vice versa, and homogenous spheres of a TiAl alloy.

MM 65.2 Thu 17:00 C 230

On the Road to Hierachically Porous Silicon by Dealloying Additively Manufactured Aluminium-Silicon Alloys — •Manfred May[1,2,3], Philipp Timm[1], Maria Mailwald[4], Dirk Herzog[5,6], Ingomar Kelbassa[5,6], and Patrick Huber[1,2,3] — [1]Hamburg University of Technology, Institute for Materials and X-Ray Physics, Hamburg, Germany — [2]DESY Centre for X-Ray and Nano Science, Hamburg, Germany — [3]Hamburg University, Center for Hybrid Nanostructures, Hamburg, Germany — [4]Hamburg University of Technology, Institute of Laser and System Technologies, Hamburg, Germany — [5]Hamburg University of Technology, Institute for Industralization of Smart Materials, Hamburg, Germany — [6]Fraunhofer, Institute of Additive Production Technologies, Hamburg, Germany

This study focuses on the synthesis of a novel hierarchically porous silicon material through a multi-step approach. Beginning with the selective laser melting fabrication of Al-Si alloys, the subsequent stages involve porosification through dealloying in HCl or KOH, creating a distinctive "coral" structure. Subsequently, another hierarchical layer is introduced via metal-assisted chemical etching or electrochemical anodic etching techniques. Different alloy compositions are investigated, and the impact of the microstructure of the 3D printed alloy for a successful dealloying process is shown. The dealloying process is checked via energy dispersive X-ray spectroscopy and X-ray diffraction experiments. Depending on the alloy composition, specificsurface areas (SSA) between 5.2 m^2/g to 48 m^2/g are achieved, with an additional increase in SSA up to 22% via anodic etching.

MM 65.3 Thu 17:15 C 230

Developing of Zr-Based Bulk Metallic Glass through Laser Powder Bed Fusion Employing Conventional and Non-Standard Beam Distributions — •Sepide Hadibeik[1], Hossein Ghasemi-Tabasi[2], Andreas Burn[3], Florian Spieckermann[4], and Jürgen Eckert[5] — [1]Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, 8700 Leoben, Austria — [2]Switzerland Innovation Park Biel/Bienne, Aarbergstrrasse 46, 2503 Biel/Bienne, Switzerland — [3]Switzerland Innovation Park Biel/Bienne, Aarbergstrrasse 46, 2503 Biel/Bienne, Switzerland — [4]Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, 8700 Leoben, Austria — [5]Erich Schmid Institute, Austrian Academy of Sciences, Jahnstraße 12, 8700 Leoben, Austria

Limitations in metallic glass additive manufacturing arise from the relaxation of solidified layers, diminishing free volume and adversely affecting part quality. Modifying the laser beam shape offers control over the molten pool’s configuration and temperature distribution, bolstering productivity. Employing an advanced beam shaping technique in laser powder bed fusion, featuring a non-Gaussian, uniform beam distribution, resulted in a shallow and broad molten pool. Analysis using pair distribution function and differential scanning calorimetry demonstrated improved amorphous structure with reduced relaxation. This non-standard beam shape induced increased free volume and enhanced atomic rearrangements, contributing to improved structural heterogeneity observed in hardness measurements.

MM 65.4 Thu 17:30 C 230

Characterization of gas-flow assisted additive manufacturing of metallic glass powders on ground and in microgravity — Mélanie Clozel[1], Christian Neumann[1], Johannes Thore[1], •Fan Yang[1], Janka Wilbig[2], Olof Gutowski[3], Ann-Christin Dippel[3], Jens Günster[2], and Andreas Meyer[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Cologne, Germany — [2]Bundesanstalt für Material-

forschung und Prüfung (BAM), 12205 Berlin, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

We studied bulk metallic glass samples produced from gas-flow assisted laser powder bed fusion process, which is capable of additively manufacture metallic parts under microgravity. The process was performed in a compact sounding rocket payload called MARS-M, in which two metallic glass alloy compositions, $Zr_{59.3}Cu_{28.8}Al_{10.4}Nb_{1.5}$ and $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ have been processed on ground and under microgravity. Using scanning electron microscopy and synchrotron X-ray diffraction tomography, we show that for both compositions the obtained samples contain given crystalline fractions, which preferably form at the interlayer boundaries. Very similar microstructures and crystalline fractions are also observed in the sample manufactured under microgravity conditions. Part of the nanocrystalline phases can be identified as the Cu_2Zr_4O phase, which might be related to the oxygen content in the initial material and the processing atmosphere. With these results, these process conditions can be improved for further space applications.

MM 65.5 Thu 17:45 C 230

Research progress for developing Fe-based soft magnetic metallic glasses for additive manufacturing — •Amirhossein Ghavimi[1], Maryam Rahimi Chegeni[1], Bastian Adam[1], Lucas Ruschel[1], Gabriele Barrera[2], Enzo Ferrara[2], Paola Tiberto[2], Isabella Gallino[3], and Ralf Busch[1] — [1]Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany — [2]INRIM, Strade delle Cacce 91, Torino, Italy — [3]Department of Materials Science and Engineering, Metallic Materials, TU-Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, Germany

This research aims to create suitable Fe-based soft magnetic amorphous alloys for the 3D printing of motor parts, based on the iron-silicon-boron (Fe-Si-B) ternary system. The goal is to enhance the glass forming ability (GFA) to achieve a fully amorphous structure in 3D-printed parts, which is expected to improve motor efficiency by increasing magnetic softness and reducing energy losses. This is achieved through adjusting the compositions while maintaining competitive soft magnetic properties.

For increasing GFA, the critical thickness of samples was examined. The structure and thermal behavior of the samples were characterized using XRD, DSC, and DTA. Magnetic properties were determined by VSM. The hysteresis loops were measured in the low and medium frequencies.

The eutectic zone of the Fe-Si-B system was experimentally determined. Evaluating quaternary and quinary component alloys involved studying the effects of elements on GFA and magnetic properties.